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The forsterite-tephroite series: I. Crystal structure refinements

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Abstract

The crystal structures of the following metamorphic olivines, $M_2^{2+}[SiO_4]$, in the forsterite-tephroite (Fo-Te) series were refined in space group *Pbnm*:

	Cation composition M				Cell parameters (Å)			
	Mg	Mn	Ca	Fe	*a*	*b*	*c*	*R factor*
Fo_{51}	1.028	0.964	0.006	0.002	4.794	10.491	6.123	0.029
Te_{91}	0.181	1.780	0.013	0.026	4.879	10.589	6.234	0.039

Treating minor Fe and Ca as though they were Mn, the refined cation distributions (*esd*'s < 0.01) and mean bond lengths are:

	M(1) site			M(2) site			
	Mg	Mn	⟨M(1)–O⟩	Mg	Mn	⟨M(2)–O⟩	⟨Si–O⟩
Fo_{51}	0.92	0.08	2.116Å	0.11	0.89	2.185Å	1.637Å
Te_{91}	0.17	0.83	2.029Å	0.00	1.00	2.227Å	1.640Å

By comparison, a previously refined synthetic $Fo_{53}Te_{47}$ specimen "heat-treated at 1000°C" is significantly more disordered ($K_D = 0.196$) than the naturally occurring Fo_{51} ($K_D = 0.011$). As expected, mean M(1)–O and M(2)–O distances correlate linearly with Mg/(Mg+Mn) occupancy.

Introduction

With the widespread availability of automated X-ray diffractometers and least-squares refinement programs, order–disorder has become a principal theme of contemporary crystal chemical investigations (Burnham, 1973). Both natural and synthetic compounds with the olivine structure have been intensively studied (for a review, see Ganguli, 1977). At least 25 different room-temperature refinements of the geologically-important Mg–Fe olivines have been carried out and 13 additional refinements extend the observational conditions to temperatures of ~1000°C and pressures of ~50 kbar (Basso *et al.*, 1979; Birle *et al.*, 1968; Brown and Prewitt, 1973; Finger, 1970; Finger and Virgo, 1971; Hazen, 1976; Smyth, 1975; Smyth and Hazen, 1973; Wenk and Raymond, 1973).

However, the crystal structures of only two Mg–Mn olivines have previously been refined. One of them contains 11 mole percent of Zn_2SiO_4, thereby complicating the octahedral site refinement (Brown, 1970). The other is synthetic $Fo_{53}Te_{47}$ which was "heat treated at 1000°C" (Ghose and Weidner, 1974; Ghose *et al.*, 1976) and thus does not represent a naturally equilibrated Mg/Mn distribution. The present refinements were undertaken to examine Mg/Mn ordering in natural olivines uncomplicated by additional substituents.

Experimental procedures and structure refinement

The crystals used for refinement were selected from the suite of specimens described in Part II of this study (in preparation). The manganoan forsterite

RFINE F051TE49 FINAL CYCLE

CONTROL PARAMETERS ARE
1 1 1 2 2 0 0 1 1 1 1 1 1 1 1 1.50 2.50 0 0 1 4 6 1 1 0 1 1 0.0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0

REAL CELL	4.79400	10.49100	6.12300	90.00000	90.00000	90.00000
RECIPROCAL CELL	0.20859	0.09532	0.16332	0.0	0.0	0.0

SYMMETRY CARDS

	X		Y		Z	0
1/2	X	1/2	-Y		-Z	0
1/2	-X	1/2	Y	1/2	-Z	0
	-X		-Y	1/2	Z	1

SCATTERING CURVES

LABEL	A(1)	B(1)	A(2)	B(2)	A(3)	B(3)	A(4)	B(4)	C	DFR	DFI
MG	5.420400	2.827499	2.173499	79.261093	1.226899	0.380800	2.307300	7.193700	0.858400	0.042	0.036
MN	11.281899	5.340899	7.357300	0.343200	3.019300	17.867386	2.244100	83.754288	1.089600	0.295	0.729
SI	6.291499	2.438600	3.035299	32.333694	1.989100	0.678500	1.540999	81.693695	1.140699	0.072	0.071
O	3.048499	13.277100	2.286799	5.701099	1.546300	0.323900	0.867000	32.908890	0.250500	0.008	0.006

SCALE FACTORS - 8.5120

EXTINCTION PARAMETERS - 0.88041E-01 0.0 0.0 0.0 0.0 0.0

ATOM LABEL	X	Y	Z	TEMPERATURE FACTOR DATA					
M1	0.0	0.0	0.0	0.00307	0.00135	0.00247	-0.00007	-0.00046	-0.00034
M2	0.9870	0.2790	0.2500	0.00612	0.00116	0.00366	0.00024	0.0	0.0
SI	0.4226	0.0910	0.2500	0.00312	0.00096	0.00252	0.00004	0.0	0.0
O1	0.7585	0.0867	0.2500	0.00220	0.00169	0.00365	-0.00016	0.0	0.0
O2	0.2300	0.4489	0.2500	0.00402	0.00112	0.00378	-0.00048	0.0	0.0
O3	0.2782	0.1590	0.0374	0.00394	0.00134	0.00362	-0.00002	-0.00004	0.00037

ATOM LABEL	TF	SCAT.		SITE	OCCUP	OCCA
M1	1	1	2	0.500	1.000	0.920
M2	1	1	2	0.500	1.000	0.109
SI	1	3	0	0.500	1.000	1.000
O1	1	4	0	0.500	1.000	1.000
O2	1	4	0	0.500	1.000	1.000
O3	1	4	0	1.000	1.000	1.000

PARAMETER SELECTION INFORMATION
1000111111011011110001101111000110111100011011110001111111l1

DEPENDENT PARAMETER INFORMATION
2 1 0 00.1030E 01 2 1100100-.1000E 01

FORMAT FOR STRUCTURE FACTOR INPUT IS
(I1,I3,2I4,2F9.4,I3,F11.6,4F7.2,A2,I6)

WAVELENGTH IS 0.7093

RFINE FO51TE49 FINAL CYCLE STRUCTURE FACTORS PAGE 1

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
0	4	0	27.183	29.941	30.242	2.047	-2.758	-40.2373	0.9758
0	6	0	15.878	17.213	-17.223	-1.051	-1.335	-15.9729	0.9952
0	8	0	11.183	10.251	10.243	0.534	0.932	8.7691	0.9989
0	10	0	32.666	32.210	32.324	1.077	0.456	4.7732	0.9919
0	12	0	25.423	26.112	26.156	-0.739	-0.689	-6.3103	0.9958
0	14	0	33.201	33.117	33.152	1.983	0.084	0.7249	0.9944
0	16	0	34.632	34.162	-34.203	-1.886	0.469	3.7754	0.9946
0	2	1	32.330	31.076	-31.578	0.651	1.254	36.8409	0.9680
0	4	1	59.314	61.596	-64.369	-1.901	-2.283	-50.8433	0.9149
0	6	1	74.574	76.247	79.776	2.325	-1.673	-31.3883	0.9127
0	8	1	7.900	8.333	-8.063	-2.114	-0.433	-5.3959	0.9993
0	10	1	56.611	56.713	57.412	2.403	-0.102	-1.5203	0.9741
0	12	1	40.345	40.184	-40.331	-1.940	0.161	2.1969	0.9904
0	14	1	14.000	14.211	-14.191	0.675	-0.211	-2.3789	0.9989
0	16	1	14.824	14.604	-14.602	-0.508	0.221	2.3666	0.9990
0	2	2	39.841	43.743	44.461	2.590	-3.902	-102.5647	0.9647
0	4	2	6.856	7.257	-7.130	-1.369	-0.401	-6.6290	0.9991
0	6	2	116.255	115.441	125.988	1.804	0.814	15.3207	0.8394
0	8	2	32.371	32.559	32.739	0.123	-0.188	-3.0353	0.9890
0	10	2	18.077	18.317	-18.333	-0.500	-0.240	-3.3434	0.9975
0	12	2	25.416	25.268	25.278	1.382	0.148	1.9193	0.9963
0	14	2	6.993	5.495	-5.316	-1.390	1.498	13.1387	0.9998
0	16	2	35.500	35.077	35.107	2.308	0.423	4.8478	0.9940
0	2	3	7.372	7.031	-7.002	-0.665	0.341	6.5804	0.9995
0	4	3	71.076	72.094	74.303	1.883	-1.018	-21.2784	0.9408
0	6	3	57.313	58.531	-59.539	-2.243	-1.218	-22.3723	0.9651
0	8	3	9.210	9.382	-9.166	2.021	-0.172	-2.2786	0.9992
0	10	3	42.723	43.142	-43.377	-2.306	-0.419	-6.0058	0.9864
0	12	3	42.091	42.554	42.734	1.912	-0.463	-6.0101	0.9896
0	14	3	5.006	4.640	4.558	-0.869	0.366	2.4897	0.9999
0	16	3	16.376	16.460	16.463	0.514	-0.084	-0.8670	0.9986
0	2	4	4.735	3.432	2.915	-1.812	1.303	17.1566	0.9999
0	4	4	31.448	31.335	31.414	1.945	0.113	2.1483	0.9912
0	6	4	22.610	22.993	-23.022	-1.006	-0.382	-6.4654	0.9956
0	8	4	10.335	9.821	9.811	0.512	0.514	5.8407	0.9993
0	10	4	30.573	30.815	30.880	1.039	-0.241	-3.2943	0.9947
0	12	4	16.546	17.336	17.337	-0.701	-0.790	-9.2735	0.9983
0	14	4	28.369	28.190	28.183	1.873	0.179	2.0383	0.9961
0	2	5	28.467	28.604	-28.676	0.565	-0.137	-2.4948	0.9946
0	4	5	31.975	31.359	-31.407	-1.721	0.615	10.7506	0.9940
0	6	5	51.847	52.196	52.557	2.145	-0.350	-5.6838	0.9847
0	8	5	14.006	14.109	-13.981	-1.950	-0.103	-1.4041	0.9989
0	10	5	46.557	46.697	46.907	2.227	-0.140	-1.8629	0.9888
0	12	5	26.991	26.959	-26.959	-1.757	0.032	0.3746	0.9958
0	14	5	16.204	16.890	-16.885	0.783	-0.686	-7.1299	0.9985
0	0	6	53.086	53.726	-54.126	-2.251	-0.640	-10.7593	0.9836
0	2	6	33.762	33.615	33.640	2.325	0.146	2.4431	0.9938
0	4	6	8.283	7.937	7.851	-1.180	0.346	4.4352	0.9996
0	6	6	61.013	61.167	61.727	1.597	-0.153	-2.3064	0.9813
0	8	6	21.346	21.330	21.358	0.127	0.016	0.2111	0.9973
0	10	6	7.360	6.769	-6.757	-0.418	0.591	5.5373	0.9998
0	12	6	12.801	12.426	12.372	1.211	0.375	3.2739	0.9991
0	2	7	3.681	3.256	-3.205	-0.576	0.425	3.3014	0.9999

RFINE F051TE49 FINAL CYCLE

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F
0	4	7	42.745		42.422	42.572	1.648	0.32
0	6	7	31.985		31.516	-31.530	-1.931	0.46
0	8	7	8.373		8.821	-8.652	1.729	-0.44
0	10	7	26.347		26.399	-26.368	-1.984	-0.05
0	12	7	31.794		31.804	31.851	1.673	-0.01
0	0	8	64.798		64.437	65.003	2.646	0.36
0	2	8	5.012		5.165	4.947	-1.484	-0.15
0	4	8	21.722		21.758	21.718	1.662	-0.03
0	6	8	22.900		22.785	-22.799	-0.871	0.11
0	8	8	6.715		6.450	6.435	0.449	0.26
0	10	8	23.994		24.540	24.564	0.921	-0.54
0	2	9	13.466		13.522	-13.520	0.451	-0.05
0	4	9	17.273		17.420	-17.376	-1.411	-0.14
0	6	9	29.641		29.283	29.287	1.757	0.35
1	1	0	11.565		12.860	-12.908	-0.323	-1.29
1	2	0	28.214		28.636	-29.087	-0.200	-0.42
1	3	0	83.674		81.038	89.437	1.734	2.63
1	4	0	59.145		56.158	58.371	0.113	2.98
1	5	0	12.033		10.549	10.467	-1.406	1.48
1	6	0	22.167		21.193	21.268	-0.109	0.97
1	7	0	86.231		87.022	91.356	2.831	-0.79
1	8	0	9.740		9.476	-9.477	0.266	0.26
1	9	0	24.754		24.565	-24.543	-2.112	0.18
1	10	0	4.037		5.058	5.057	-0.114	-1.02
1	11	0	30.839		30.861	30.891	2.127	-0.02
1	12	0	4.702		1.574	1.571	0.104	3.12
1	13	0	13.757		13.451	-13.397	-1.281	0.30
1	14	0	19.098		19.597	-19.616	-0.250	-0.49
1	15	0	28.838		29.230	29.268	1.190	-0.39
1	16	0	1.689	*	0.279	-0.278	0.024	1.40
1	0	1	27.732		26.269	-26.477	0.068	1.46
1	1	1	54.403		55.118	-56.809	-2.397	-0.71
1	2	1	17.413		17.277	-17.325	-0.254	0.13
1	3	1	84.635		86.121	91.926	2.421	-1.48
1	4	1	3.451		4.275	4.270	0.230	-0.82
1	5	1	31.558		32.727	-32.942	-1.468	-1.16
1	6	1	4.463		4.033	-4.033	-0.001	0.43
1	7	1	5.858		5.026	-4.999	0.525	0.83
1	8	1	7.922		8.686	8.689	0.061	-0.76
1	9	1	16.461		16.558	-16.579	-0.039	-0.09
1	10	1	8.376		8.353	8.355	-0.022	0.02
1	11	1	13.798		14.171	-14.150	-0.945	-0.37
1	12	1	1.983		0.307	-0.260	-0.164	1.67
1	13	1	34.958		34.480	34.558	1.721	0.47
1	14	1	5.032		4.745	4.743	0.155	0.28
1	15	1	11.936		11.494	-11.376	-1.670	0.44
1	16	1	1.043	*	0.780	0.777	-0.062	0.26
1	1	2	75.692		73.929	77.230	1.027	1.76
1	2	2	49.492		46.073	-46.725	0.118	3.41
1	3	2	6.075		4.225	4.109	-0.985	1.85
1	4	2	1.573		0.834	0.833	-0.046	0.73
1	5	2	46.219		47.563	48.256	2.074	-1.34
1	6	2	3.999		4.209	-4.207	0.132	-0.21

RFINE F051TE49 FINAL CYCLE STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	7	2	37.387		38.635	-38.904	-2.130	-1.248	-21.0112	0.9832	
1	8	2	28.397		29.123	-29.250	-0.342	-0.726	-11.1726	0.9912	
1	9	2	68.366		68.893	70.271	2.738	-0.527	-7.9358	0.9597	
1	10	2	10.472		10.696	10.700	0.154	-0.224	-2.7078	0.9992	
1	11	2	4.176		4.275	4.009	-1.486	-0.099	-0.6944	0.9999	
1	12	2	11.355		11.496	11.501	-0.061	-0.141	-1.5513	0.9992	
1	13	2	35.270		35.245	35.333	1.823	0.025	0.3128	0.9924	
1	14	2	0.876	*	0.372	-0.324	0.182	0.504	0.7109	1.0000	* **
1	15	2	5.950		5.493	-5.457	-0.635	0.456	3.4015	0.9999	
1	16	2	4.982		4.650	4.650	-0.006	0.333	2.2031	0.9999	
1	0	3	12.864		11.740	-11.748	-0.104	1.124	24.1847	0.9985	
1	1	3	47.826		48.140	48.720	2.334	-0.314	-7.1828	0.9741	
1	2	3	26.147		25.363	25.455	0.265	0.784	17.1810	0.9927	
1	3	3	72.749		72.086	-73.817	-2.350	0.663	14.0116	0.9527	
1	4	3	11.697		11.067	11.071	-0.197	0.630	11.4720	0.9989	
1	5	3	22.334		23.134	23.155	1.423	-0.800	-14.8018	0.9944	
1	6	3	16.366		17.259	-17.279	-0.036	-0.893	-14.9702	0.9977	
1	7	3	7.712		7.592	7.577	-0.497	0.120	1.4984	0.9996	
1	8	3	4.958		4.794	-4.794	-0.052	0.163	1.5767	0.9998	
1	9	3	16.181		16.514	16.532	0.050	-0.333	-4.5569	0.9978	
1	10	3	3.109		3.422	3.422	0.053	-0.313	-1.8345	0.9999	
1	11	3	11.186		11.245	11.212	0.920	-0.060	-0.6992	0.9992	
1	12	3	8.286		8.515	-8.516	0.133	-0.228	-2.1978	0.9996	
1	13	3	30.481		30.549	-30.590	-1.661	-0.067	-0.8035	0.9944	
1	14	3	5.821		5.372	-5.370	-0.153	0.450	3.3191	0.9999	
1	15	3	12.543		12.216	12.110	1.635	0.327	3.2208	0.9993	
1	16	3	6.339		6.486	6.486	0.087	-0.147	-1.0653	0.9998	
1	1	4	5.278		5.266	-5.258	-0.300	0.013	0.1751	0.9998	
1	2	4	8.383		8.552	-8.553	-0.174	-0.169	-2.7158	0.9994	
1	3	4	57.840		57.120	57.911	1.640	0.721	13.8656	0.9721	
1	4	4	22.265		22.506	22.546	0.091	-0.241	-4.3609	0.9964	
1	5	4	11.566		11.024	10.950	-1.315	0.542	8.5255	0.9992	
1	6	4	11.140		11.560	11.566	-0.106	-0.420	-6.2587	0.9989	
1	7	4	68.410		68.958	70.178	2.681	-0.548	-8.8905	0.9641	
1	8	4	1.805		1.194	1.163	0.270	0.611	2.4885	1.0000	
1	9	4	20.811		21.023	-20.961	-1.990	-0.212	-2.9290	0.9969	
1	10	4	1.718		1.045	1.039	-0.116	0.673	2.3096	1.0000	
1	11	4	24.666		24.984	24.954	2.008	-0.319	-4.0140	0.9960	
1	12	4	1.494	*	0.840	-0.835	0.089	0.655	1.6788	1.0000	* **
1	13	4	11.201		11.134	-11.072	-1.202	0.068	0.6836	0.9993	
1	14	4	12.681		13.085	-13.089	-0.224	-0.403	-3.9987	0.9991	
1	15	4	24.444		24.731	24.749	1.127	-0.287	-3.0428	0.9964	
1	0	5	27.132		27.291	-27.358	0.031	-0.159	-2.8715	0.9951	
1	1	5	28.039		27.811	-27.797	-2.187	0.229	4.1187	0.9948	
1	2	5	4.198		3.916	-3.910	-0.220	0.281	2.7368	0.9999	
1	3	5	57.013		56.167	56.675	2.227	0.846	14.8127	0.9806	
1	4	5	13.000		13.180	13.185	0.233	-0.180	-2.8274	0.9990	
1	5	5	20.509		20.896	-20.884	-1.344	-0.387	-6.2562	0.9970	
1	6	5	9.975		10.208	-10.211	-0.023	-0.232	-3.1739	0.9993	
1	7	5	3.559		3.102	-3.064	0.486	0.457	3.3520	0.9999	
1	8	5	7.061		7.096	7.096	0.061	-0.034	-0.3696	0.9997	
1	9	5	11.131		11.436	-11.441	-0.031	-0.306	-3.6155	0.9992	
1	10	5	12.174		12.485	12.490	0.000	-0.311	-3.5496	0.9992	

RFINE F051TE49 FINAL CYCLE

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	11	5	11.809	11.749	-11.722	-0.861	0.060	0.6510	0.9992	
1	12	5	5.745	5.890	-5.888	-0.172	-0.145	-1.0708	0.9998	
1	13	5	27.769	28.101	28.115	1.593	-0.332	-3.7393	0.9958	
1	14	5	3.837	3.048	3.045	0.140	0.789	4.1515	0.9999	
1	1	6	44.623	43.756	43.982	0.936	0.867	14.3552	0.9893	
1	2	6	4.230	3.530	-3.527	0.136	0.700	6.4276	0.9999	
1	3	6	1.647	1.118	-0.702	-0.870	0.529	2.1503	1.0000	
1	4	6	5.837	5.790	-5.791	-0.060	0.046	0.4976	0.9998	
1	5	6	26.077	25.883	25.861	1.851	0.194	2.9496	0.9966	
1	6	6	4.912	4.904	-4.903	0.109	0.008	0.0777	0.9999	
1	7	6	23.793	23.899	-23.864	-1.884	-0.106	-1.4750	0.9967	
1	8	6	10.218	10.008	-10.007	-0.281	0.210	2.4005	0.9994	
1	9	6	44.540	44.746	44.898	2.445	-0.206	-2.6755	0.9903	
1	10	6	2.948	2.847	2.844	0.120	0.101	0.4789	1.0000	
1	11	6	1.894	2.284	1.876	-1.303	-0.390	-1.1880	1.0000	
1	12	6	5.464	5.023	5.023	-0.064	0.441	2.9894	0.9999	
1	13	6	26.214	26.958	26.959	1.638	-0.744	-8.0289	0.9962	
1	0	7	6.662	6.512	-6.512	-0.097	0.150	1.6752	0.9998	
1	1	7	23.454	23.053	22.995	2.014	0.401	5.8938	0.9974	
1	2	7	13.875	13.640	13.645	0.238	0.235	3.2019	0.9991	
1	3	7	40.570	39.938	-40.049	-2.036	0.632	9.1840	0.9919	
1	4	7	6.306	6.126	6.125	-0.163	0.179	1.7925	0.9998	
1	5	7	11.946	11.826	11.766	1.229	0.120	1.4986	0.9993	
1	6	7	13.619	13.687	-13.694	-0.047	-0.068	-0.8425	0.9990	
1	7	7	5.505	5.524	5.509	-0.415	-0.019	-0.1569	0.9999	
1	8	7	2.484	2.499	-2.499	-0.044	-0.016	-0.0686	1.0000	
1	9	7	11.506	10.964	10.967	0.060	0.542	5.7663	0.9994	
1	10	7	5.489	5.036	5.036	0.061	0.453	3.4227	0.9999	
1	11	7	8.036	7.447	7.404	0.801	0.590	5.0949	0.9997	
1	1	8	3.452	3.336	-3.327	-0.241	0.116	0.7289	0.9999	
1	2	8	3.396	3.666	3.665	-0.122	-0.271	-1.6365	0.9999	
1	3	8	27.803	27.222	27.235	1.388	0.581	7.5717	0.9965	
1	4	8	3.414	2.740	2.739	0.047	0.674	4.1237	1.0000	
1	5	8	5.825	6.133	6.038	-1.074	-0.308	-2.6312	0.9998	
1	6	8	4.081	3.797	3.796	-0.096	0.284	1.8012	0.9999	
1	7	8	40.395	40.767	40.876	2.277	-0.372	-4.5690	0.9916	
1	8	8	8.677	8.731	8.729	0.262	-0.054	-0.5089	0.9996	
1	9	8	15.624	15.177	-15.094	-1.663	0.447	4.7210	0.9989	
1	0	9	12.906	12.686	-12.690	0.022	0.220	2.4850	0.9993	
1	1	9	14.671	14.305	-14.201	-1.774	0.366	4.1551	0.9991	
1	2	9	2.736	2.462	-2.455	-0.182	0.273	1.2519	1.0000	
1	3	9	30.032	29.794	29.798	1.829	0.238	2.8612	0.9959	
1	4	9	6.886	6.717	6.715	0.194	0.170	1.4630	0.9998	
1	5	9	11.508	11.357	-11.309	-1.087	0.150	1.5671	0.9994	
1	6	9	5.356	5.311	-5.312	-0.009	0.045	0.3260	0.9999	
2	0	0	39.681	44.074	44.627	2.943	-4.393	-79.6876	0.9711	
2	1	0	39.419	38.912	39.703	0.545	0.508	9.4471	0.9603	
2	2	0	24.955	26.354	-26.502	-1.926	-1.399	-17.9446	0.9837	
2	3	0	19.333	19.616	19.696	-0.125	-0.283	-3.4411	0.9919	
2	4	0	86.470	84.219	89.988	2.125	2.251	27.0724	0.8754	
2	5	0	1.180 *	0.335	0.151	0.299	0.845	1.4150	1.0000	* **
2	6	0	17.161	17.232	-17.243	-0.918	-0.071	-0.7147	0.9959	
2	7	0	18.853	17.634	-17.665	-0.291	1.218	12.0578	0.9963	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
2	8	0	40.024		39.404	39.712	0.597	0.619	6.3237	0.9844	
2	9	0	17.085		16.989	-17.009	-0.199	0.096	0.8873	0.9975	
2	10	0	53.427		51.984	52.521	1.042	1.443	13.8482	0.9793	
2	11	0	1.611	*	2.507	-2.504	0.120	-0.896	-1.7956	1.0000	* **
2	12	0	4.230		4.600	-4.519	-0.860	-0.370	-1.6449	0.9999	
2	13	0	13.010		12.773	12.779	-0.035	0.237	1.7664	0.9991	
2	14	0	29.601		28.764	28.764	1.922	[illegible]	6.7975	0.9956	
2	15	0	15.543		15.538	15.542	0.438	[illegible]	0.0340	0.9988	
2	16	0	10.064		8.578	-8.419	-1.654	1.486	9.4447	0.9996	
2	1	1	32.045		31.581	31.820	0.132	0.464	11.1708	0.9850	
2	2	1	18.456		18.259	18.294	0.765	0.197	4.2723	0.9945	
2	3	1	1.210		0.813	0.795	0.173	0.397	1.7085	1.0000	
2	4	1	56.276		57.891	-59.422	-1.768	-1.614	-30.3759	0.9483	
2	5	1	31.292		31.702	-31.883	-0.526	-0.410	-7.0242	0.9884	
2	6	1	33.881		34.132	34.280	2.157	-0.251	-4.0208	0.9875	
2	7	1	8.392		8.853	-8.854	0.222	-0.461	-5.3865	0.9992	
2	8	1	36.183		36.439	-36.607	-2.186	-0.256	-3.7591	0.9873	
2	9	1	1.081	*	1.234	-1.198	-0.293	-0.153	-0.3160	1.0000	* **
2	10	1	33.644		32.947	33.021	2.220	0.698	9.2212	0.9910	
2	11	1	20.596		20.209	20.230	0.538	0.387	4.7854	0.9973	
2	12	1	24.626		24.476	-24.459	-1.785	0.149	1.8019	0.9961	
2	13	1	3.285		2.741	2.736	-0.172	0.544	2.6771	1.0000	
2	14	1	17.511		17.238	17.221	1.018	0.274	2.9360	0.9984	
2	15	1	6.305		6.191	-6.191	0.026	0.115	0.8463	0.9998	
2	16	1	1.172	*	0.417	-0.058	-0.413	0.755	1.2881	1.0000	* **
2	0	2	40.242		41.088	-41.405	-2.272	-0.846	-19.8394	0.9818	
2	1	2	15.032		15.478	-15.489	-0.512	-0.446	-9.7236	0.9975	
2	3	2	15.037		15.275	-15.297	0.127	-0.239	-4.7188	0.9971	
2	4	2	14.187		12.887	12.822	-1.344	1.300	23.4816	0.9980	
2	5	2	16.797		17.019	-17.044	-0.322	-0.222	-3.7821	0.9967	
2	6	2	29.057		28.529	28.614	1.507	0.528	8.7443	0.9913	
2	7	2	24.925		25.457	25.539	0.307	-0.532	-8.2388	0.9935	
2	8	2	10.284		10.412	10.416	0.074	-0.128	-1.5872	0.9992	
2	9	2	20.270		20.790	20.822	0.210	-0.520	-7.1222	0.9968	
2	10	2	7.392		6.933	6.926	-0.344	0.459	4.5771	0.9997	
2	11	2	6.702		6.162	-6.162	-0.142	0.539	4.8342	0.9997	
2	12	2	14.774		14.312	14.254	1.376	0.462	5.1269	0.9988	
2	13	2	9.212		9.263	-9.266	0.045	-0.051	-0.4780	0.9995	
2	14	2	9.668		8.824	-8.721	-1.358	0.844	7.5026	0.9995	
2	15	2	11.253		10.808	-10.804	-0.414	0.445	4.1480	0.9994	
2	16	2	40.507		40.128	40.240	2.190	0.379	4.0539	0.9915	
2	1	3	21.162		20.984	-21.024	-0.120	0.178	3.6842	0.9962	
2	2	3	8.480		8.066	8.038	-0.706	0.413	7.0296	0.9995	
2	3	3	8.312		8.201	-8.202	-0.179	0.110	1.7902	0.9995	
2	4	3	34.634		34.596	34.712	1.694	0.038	0.7086	0.9910	
2	5	3	29.738		30.051	30.146	0.520	-0.312	-5.4827	0.9934	
2	6	3	34.087		34.376	-34.455	-2.099	-0.289	-4.8148	0.9917	
2	7	3	12.004		12.411	12.417	-0.202	-0.407	-5.7140	0.9987	
2	8	3	43.922		45.132	45.383	2.163	-1.210	-18.2065	0.9868	
2	9	3	3.473		3.168	-3.156	0.275	0.305	2.0271	0.9999	
2	10	3	35.111		35.557	-35.630	-2.167	-0.446	-5.9395	0.9922	
2	11	3	17.958		18.223	-18.234	-0.522	-0.265	-3.1761	0.9980	
2	12	3	18.361		18.025	17.960	1.728	0.336	3.8482	0.9981	

RFINE F051TE49 FINAL CYCLE

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
2	13	3	1.138 *	0.524	0.493	0.178	0.613	1.0781	1.0000	* **
2	14	3	8.357	7.916	-7.860	-0.949	0.441	3.6527	0.9997	
2	15	3	4.039	3.647	3.647	-0.030	0.392	2.0624	0.9999	
2	0	4	53.934	52.758	53.243	2.802	1.176	22.8458	0.9791	
2	1	4	23.665	23.647	23.689	0.511	0.018	0.3444	0.9960	
2	2	4	18.489	19.147	-19.087	-1.816	-0.657	-11.9086	0.9973	
2	3	4	14.811	15.441	15.453	-0.115	-0.630	-10.7035	0.9984	
2	4	4	55.362	55.286	55.901	1.998	0.076	1.3444	0.9769	
2	5	4	4.445	4.388	4.379	0.289	0.057	0.5471	0.9999	
2	6	4	6.973	6.911	-6.860	-0.846	0.062	0.7263	0.9996	
2	7	4	15.548	15.975	-15.985	-0.281	-0.428	-6.1330	0.9985	
2	8	4	28.249	28.977	29.055	0.566	-0.727	-10.5034	0.9943	
2	9	4	14.528	14.718	-14.726	-0.193	-0.190	-2.4320	0.9988	
2	10	4	37.628	38.339	38.482	0.978	-0.710	-9.2721	0.9919	
2	11	4	1.080 *	0.453	-0.437	0.118	0.627	1.1618	1.0000	* **
2	12	4	1.426 *	1.115	-0.785	-0.792	0.311	0.7038	1.0000	* **
2	13	4	9.794	10.104	10.107	-0.032	-0.309	-2.8466	0.9994	
2	14	4	25.095	25.173	25.148	1.819	-0.078	-0.8284	0.9968	
2	1	5	22.562	22.445	22.480	0.134	0.117	1.9983	0.9969	
2	2	5	18.102	18.404	18.408	0.724	-0.302	-5.0326	0.9980	
2	3	5	3.276	3.797	-3.794	0.150	-0.521	-4.0840	0.9999	
2	4	5	45.541	45.406	-45.677	-1.639	0.135	2.2198	0.9869	
2	5	5	21.332	21.213	-21.233	-0.482	0.119	1.8212	0.9976	
2	6	5	22.307	21.981	21.925	1.974	0.326	4.8226	0.9970	
2	7	5	4.241	4.114	-4.108	0.209	0.128	1.0230	0.9999	
2	8	5	16.587	16.561	-16.458	-1.967	0.026	0.3469	0.9983	
2	9	5	3.617	3.204	-3.192	-0.272	0.413	2.6331	0.9999	
2	10	5	21.252	21.395	21.328	2.030	-0.143	-1.7530	0.9973	
2	11	5	15.224	15.533	15.535	0.500	-0.309	-3.3850	0.9988	
2	12	5	22.125	22.387	-22.356	-1.640	-0.262	-2.8847	0.9974	
2	13	5	3.988	4.120	4.118	-0.146	-0.132	-0.7067	0.9999	
2	0	6	14.850	14.421	-14.291	-1.985	0.429	6.3763	0.9989	
2	1	6	14.185	14.171	-14.171	-0.468	0.014	0.2100	0.9990	
2	2	6	53.969	53.718	54.076	2.346	0.251	4.0032	0.9849	
2	3	6	11.354	11.610	-11.614	0.105	-0.255	-3.5123	0.9993	
2	4	6	2.033	1.502	0.905	-1.198	0.531	2.4365	1.0000	
2	5	6	7.184	7.019	-7.014	-0.279	0.165	1.8256	0.9997	
2	6	6	28.427	28.503	28.526	1.383	-0.076	-1.0619	0.9961	
2	7	6	14.517	14.526	14.532	0.272	-0.009	-0.1117	0.9988	
2	8	6	5.022	5.124	5.124	0.074	-0.101	-0.7828	0.9999	
2	9	6	13.188	13.197	13.201	0.190	-0.009	-0.1004	0.9992	
2	10	6	4.564	1.481	-1.447	-0.320	3.083	20.8754	1.0000	
2	11	6	2.732	2.071	-2.068	-0.117	0.661	2.7259	1.0000	
2	12	6	15.538	15.828	15.789	1.251	-0.290	-2.9390	0.9986	
2	1	7	11.512	11.502	-11.505	-0.106	0.010	0.1295	0.9994	
2	2	7	8.366	8.245	8.225	-0.590	0.121	1.4104	0.9997	
2	3	7	5.176	5.040	-5.038	-0.156	0.136	1.2252	0.9999	
2	4	7	18.018	17.848	17.801	1.462	0.170	2.2573	0.9985	
2	5	7	18.658	18.437	18.446	0.461	0.222	2.8718	0.9983	
2	6	7	22.152	21.838	-21.786	-1.814	0.314	3.9990	0.9978	
2	7	7	8.667	8.726	8.726	-0.163	-0.059	-0.5881	0.9997	
2	8	7	32.043	32.155	32.177	1.881	-0.112	-1.3809	0.9952	
2	9	7	2.327	2.912	-2.903	0.232	-0.585	-2.1345	1.0000	

RFINE F051TE49 FINAL CYCLE

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
2	10	7	24.573	25.262	-25.232	-1.872	-0.689	-7.6866	0.9969	
2	11	7	11.609	12.103	-12.099	-0.457	-0.495	-4.6362	0.9993	
2	0	8	39.055	38.550	38.610	2.406	0.505	6.7454	0.9930	
2	1	8	10.093	9.831	9.824	0.425	0.262	2.9279	0.9996	
2	2	8	14.553	14.238	-14.163	-1.517	0.316	3.8782	0.9991	
2	3	8	8.208	8.432	8.433	-0.088	-0.224	-2.2937	0.9997	
2	4	8	23.722	23.752	23.723	1.668	-0.029	-0.3682	0.9974	
2	5	8	5.547	5.660	5.654	0.256	-0.112	-0.8821	0.9999	
2	6	8	3.114	3.071	2.996	-0.671	0.043	0.2128	1.0000	
2	7	8	11.181	11.301	-11.302	-0.251	-0.120	-1.2355	0.9994	
2	8	8	15.072	15.070	15.872	0.485	-0.798	-8.4623	0.9988	
2	1	9	11.872	11.722	11.725	0.121	0.150	1.6212	0.9994	
2	2	9	9.574	9.349	9.333	0.583	0.225	2.2285	0.9996	
2	3	9	0.695 *	1.707	-1.703	0.124	-1.012	-1.1845	1.0000	* **
2	4	9	24.517	24.464	-24.462	-1.336	0.053	0.6085	0.9972	
2	5	9	11.725	11.627	-11.623	-0.402	0.098	0.9953	0.9994	
3	1	0	30.476	29.266	29.488	-0.090	1.211	18.3359	0.9850	
3	2	0	30.611	30.560	-30.791	-0.452	0.052	0.5549	0.9848	
3	3	0	44.876	44.771	45.436	1.575	0.104	1.1074	0.9698	
3	4	0	51.705	50.912	-51.863	0.110	0.794	8.2697	0.9637	
3	5	0	3.144	2.569	-2.111	-1.465	0.575	2.0304	0.9999	
3	6	0	14.795	14.547	-14.558	-0.452	0.248	2.0449	0.9975	
3	7	0	70.263	66.269	67.759	2.537	3.994	37.9662	0.9552	
3	8	0	51.604	49.302	49.850	0.851	2.302	21.1957	0.9779	
3	9	0	27.247	25.920	-25.922	-1.900	1.327	11.5916	0.9945	
3	10	0	3.090	2.384	2.351	-0.391	0.707	2.3565	1.0000	
3	11	0	36.275	34.734	34.808	2.150	1.541	12.0002	0.9920	
3	12	0	6.742	6.664	-6.659	0.293	0.077	0.4143	0.9997	
3	13	0	3.601	2.602	-2.365	-1.083	0.999	3.3180	1.0000	
3	14	0	8.332	8.276	-8.263	-0.488	0.056	0.3144	0.9996	
3	15	0	15.956	15.017	14.993	0.985	0.940	6.4471	0.9988	
3	0	1	13.376	12.886	-12.891	0.331	0.491	9.7602	0.9985	
3	1	1	49.400	49.345	-49.918	-2.331	0.055	1.1209	0.9750	
3	2	1	22.919	22.918	-22.979	-0.666	0.001	0.0119	0.9939	
3	3	1	49.633	50.541	51.290	2.059	-0.909	-16.0804	0.9694	
3	4	1	34.142	34.500	34.690	0.636	-0.357	-5.8871	0.9887	
3	5	1	18.331	18.839	-18.818	-1.393	-0.507	-7.3712	0.9967	
3	6	1	30.497	30.224	30.380	-0.002	0.273	3.9586	0.9898	
3	7	1	9.210	9.520	9.503	0.628	-0.310	-3.3944	0.9992	
3	8	1	1.371 *	0.306	0.285	0.112	1.065	2.5998	1.0000	* **
3	9	1	3.384	0.617	-0.602	0.136	2.766	14.7784	1.0000	
3	10	1	29.029	28.155	-28.234	-0.144	0.873	10.3805	0.9945	
3	11	1	12.277	11.307	-11.278	-0.881	0.970	9.8059	0.9991	
3	12	1	25.745	24.475	-24.513	-0.488	1.270	14.1364	0.9965	
3	13	1	18.065	17.161	17.116	1.439	0.904	9.4517	0.9982	
3	14	1	5.236	4.620	4.602	0.402	0.616	3.9345	0.9999	
3	15	1	20.535	19.495	-19.443	-1.683	1.040	10.5699	0.9979	
3	1	2	44.421	43.502	43.846	0.812	0.919	18.3700	0.9840	
3	2	2	65.219	65.442	66.506	0.514	-0.223	-4.3065	0.9682	
3	3	2	11.283	11.336	-11.305	-0.903	-0.052	-0.8422	0.9990	
3	4	2	19.627	19.689	19.726	-0.161	-0.062	-1.0441	0.9963	
3	5	2	54.331	54.966	55.549	2.132	-0.635	-10.4761	0.9777	
3	6	2	4.435	4.418	4.398	0.426	0.017	0.1475	0.9999	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	7	2	9.408		9.701	-9.534	-1.813	-0.293	-3.4264	0.9992	
3	8	2	21.534		21.438	-21.459	-0.770	0.096	1.2700	0.9968	
3	9	2	46.591		46.150	46.419	2.464	0.441	5.7533	0.9857	
3	10	2	13.094		13.509	-13.512	0.352	-0.415	-4.5575	0.9988	
3	11	2	6.455		5.720	-5.514	-1.524	0.735	5.8205	0.9998	
3	12	2	3.854		3.554	-3.540	-0.319	0.300	1.5124	0.9999	
3	13	2	34.662		33.815	33.880	1.657	0.848	9.2306	0.9938	
3	14	2	23.557		23.376	23.403	0.542	0.181	1.3705	0.9972	
3	15	2	3.973		2.778	-2.737	-0.478	1.195	5.9998	1.0000	
3	0	3	30.548		30.060	30.158	-0.281	0.488	9.0821	0.9934	
3	1	3	33.859		33.677	33.736	2.248	0.182	3.4189	0.9921	
3	2	3	13.858		13.469	13.462	0.637	0.389	6.5365	0.9988	
3	3	3	44.680		44.355	-44.655	-2.000	0.325	5.7427	0.9846	
3	4	3	39.239		39.420	-39.658	-0.637	-0.182	-3.1060	0.9878	
3	5	3	24.342		24.749	24.770	1.376	-0.407	-6.5088	0.9952	
3	6	3	14.370		14.172	-14.180	0.035	0.198	2.8308	0.9988	
3	7	3	12.186		12.663	-12.656	-0.616	-0.477	-6.1655	0.9988	
3	8	3	2.374		1.922	-1.919	-0.111	0.452	2.0639	1.0000	
3	9	3	2.036		1.466	-1.461	-0.131	0.569	2.0897	1.0000	
3	10	3	18.009		17.973	17.990	0.121	0.036	0.4143	0.9981	
3	11	3	16.658		15.889	15.877	0.881	0.769	8.4143	0.9985	
3	12	3	29.567		29.558	29.631	0.503	0.009	0.0950	0.9948	
3	13	3	18.008		17.530	-17.490	-1.395	0.478	4.9208	0.9983	
3	14	3	3.686		3.388	-3.367	-0.385	0.298	1.3384	0.9999	
3	1	4	18.757		18.303	18.321	-0.084	0.455	7.6794	0.9979	
3	2	4	30.718		30.469	-30.556	-0.444	0.249	4.2851	0.9941	
3	3	4	38.890		38.170	38.323	1.501	0.720	12.2019	0.9905	
3	4	4	32.425		32.677	-32.794	0.112	-0.252	-4.0929	0.9929	
3	5	4	3.045		3.218	-2.909	-1.377	-0.173	-1.1588	0.9999	
3	6	4	9.141		9.045	-9.038	-0.421	0.096	1.1689	0.9995	
3	7	4	50.271		50.665	50.961	2.393	-0.394	-5.6570	0.9863	
3	8	4	35.024		35.439	35.572	0.793	-0.415	-5.6001	0.9920	
3	9	4	19.541		19.259	-19.199	-1.778	0.281	3.4431	0.9977	
3	10	4	4.201		4.312	4.297	-0.358	-0.111	-0.6735	0.9999	
3	11	4	28.809		29.084	29.087	2.032	-0.275	-3.1503	0.9949	
3	12	4	3.994		3.835	-3.825	0.281	0.159	0.8351	0.9999	
3	13	4	4.962		4.191	-4.065	-1.023	0.771	4.6927	0.9999	
3	14	4	9.951		9.947	-9.938	-0.476	0.004	0.0372	0.9994	
3	0	5	1.049	*	1.471	-1.435	0.325	-0.422	-1.0978	1.0000	* **
3	1	5	36.843		36.740	-36.811	-2.146	0.104	1.6762	0.9928	
3	2	5	19.968		19.740	-19.751	-0.620	0.228	3.5410	0.9979	
3	3	5	33.657		33.059	33.100	1.887	0.598	9.3936	0.9943	
3	4	5	18.733		18.457	18.466	0.574	0.276	4.0835	0.9981	
3	5	5	8.906		8.498	-8.406	-1.258	0.408	4.9816	0.9996	
3	6	5	29.354		29.602	29.677	0.031	-0.247	-3.4871	0.9949	
3	7	5	5.532		4.214	4.175	0.572	1.319	11.6104	0.9999	
3	8	5	2.255		0.544	-0.534	0.104	1.712	7.1771	1.0000	
3	9	5	2.187		1.771	-1.767	0.125	0.416	1.4972	1.0000	
3	10	5	25.929		26.786	-26.840	-0.153	-0.857	-9.8685	0.9959	
3	11	5	5.439		5.196	-5.136	-0.786	0.243	1.6253	0.9999	
3	12	5	14.789		14.599	-14.601	-0.431	0.190	1.8489	0.9989	
3	13	5	13.280		13.132	13.071	1.323	0.148	1.3807	0.9991	
3	1	6	23.641		23.071	23.091	0.727	0.571	8.3437	0.9973	

RFINE F051TE49 FINAL CYCLE

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	2	6	31.963	31.374	31.448	0.442	0.588	8.6696	0.9951	
3	3	6	2.526	1.894	-1.727	-0.776	0.632	3.2863	1.0000	
3	4	6	18.867	19.053	19.070	-0.117	-0.186	-2.5569	0.9982	
3	5	6	33.292	33.372	33.405	1.903	-0.080	-1.1012	0.9948	
3	6	6	4.685	4.547	4.531	0.383	0.138	1.0282	0.9999	
3	7	6	10.793	10.522	-10.401	-1.612	0.271	3.0200	0.9994	
3	8	6	21.339	21.581	-21.593	-0.716	-0.242	-2.9172	0.9978	
3	9	6	35.822	35.837	35.893	2.216	-0.015	-0.1775	0.9931	
3	10	6	5.701	6.122	-6.114	0.322	-0.421	-2.9795	0.9998	
3	11	6	5.618	5.181	-5.004	-1.345	0.437	2.8937	0.9999	
3	0	7	21.418	21.318	21.341	-0.216	0.100	1.3257	0.9978	
3	1	7	18.468	18.098	18.008	1.936	0.370	4.8303	0.9984	
3	2	7	7.684	7.357	7.337	0.554	0.327	3.3586	0.9997	
3	3	7	26.649	26.293	-26.279	-1.727	0.356	4.7031	0.9968	
3	4	7	25.686	25.651	-25.684	-0.561	0.034	0.4453	0.9970	
3	5	7	17.198	17.204	17.174	1.199	-0.006	-0.0780	0.9987	
3	6	7	5.619	5.838	-5.838	0.034	-0.219	-1.7158	0.9998	
3	7	7	8.992	9.091	-9.077	-0.529	-0.098	-0.9418	0.9996	
3	8	7	1.021 *	1.375	-1.372	-0.095	-0.354	-0.5968	1.0000	* **
3	9	7	3.183	1.632	-1.629	-0.108	1.551	7.3033	1.0000	
3	10	7	9.292	9.705	9.707	0.107	-0.413	-3.5974	0.9995	
3	1	8	6.698	6.718	6.718	-0.064	-0.020	-0.1763	0.9998	
3	2	8	24.347	24.439	-24.470	-0.409	-0.093	-1.1322	0.9972	
3	3	8	25.496	25.695	25.700	1.292	-0.199	-2.4184	0.9971	
3	4	8	12.743	13.022	-13.026	0.106	-0.279	-3.0023	0.9992	
3	5	8	4.708	4.268	-4.113	-1.142	0.440	2.9949	0.9999	
3	6	8	4.003	3.821	-3.805	-0.342	0.183	1.0368	0.9999	
3	7	8	28.247	28.220	28.201	2.012	0.027	0.2980	0.9963	
3	0	9	1.763	0.697	-0.649	0.252	1.067	3.0715	1.0000	
3	1	9	21.210	20.781	-20.727	-1.746	0.429	4.8245	0.9981	
3	2	9	10.793	10.682	-10.673	-0.506	0.110	1.0750	0.9995	
4	0	0	91.480	90.902	93.572	2.569	0.578	7.5400	0.9430	
4	1	0	16.391	16.057	16.061	0.858	0.334	4.0381	0.9967	
4	2	0	12.595	12.260	-12.144	-1.770	0.335	2.6864	0.9981	
4	3	0	12.284	12.240	12.244	-0.400	0.044	0.3463	0.9982	
4	4	0	45.436	43.738	44.168	2.012	1.697	15.4582	0.9786	
4	5	0	29.521	28.542	28.663	0.572	0.979	8.4612	0.9912	
4	6	0	14.763	13.698	13.700	-0.554	1.065	7.9911	0.9981	
4	7	0	22.124	21.297	-21.338	-0.422	0.827	6.5179	0.9958	
4	8	0	12.539	11.972	11.968	0.525	0.567	3.9162	0.9988	
4	9	0	18.555	17.403	-17.422	-0.227	1.152	8.5540	0.9977	
4	10	0	6.823	6.177	6.137	0.712	0.646	3.6390	0.9997	
4	11	0	10.492	10.136	10.136	0.268	0.356	2.2049	0.9993	
4	12	0	2.634	1.974	1.770	-0.872	0.660	1.6601	1.0000	
4	13	0	2.821	1.590	1.572	-0.238	1.231	3.3282	1.0000	
4	14	0	29.319	27.816	27.820	1.780	1.503	10.7107	0.9957	
4	1	1	10.262	10.040	10.044	0.061	0.222	3.3680	0.9992	
4	2	1	16.508	16.114	16.109	0.871	0.394	6.1029	0.9977	
4	3	1	3.846	3.570	3.553	0.344	0.276	2.1957	0.9999	
4	4	1	14.905	15.366	-15.321	-1.387	-0.461	-6.2777	0.9977	
4	5	1	29.248	29.518	-29.607	-0.799	-0.270	-3.7097	0.9933	
4	[illegible]	1	36.244	36.150	36.282	1.907	0.094	1.2372	0.9900	
4	7	1	1.796	1.194	-1.073	0.525	0.602	1.7049	1.0000	

RFINE F051TE49 FINAL CYCLE

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
4	8	1	30.277	29.373	-29.391	-2.133	0.904	10.7833	0.9935	
4	9	1	3.130	2.758	2.697	-0.575	0.372	1.7480	0.9999	
4	10	1	28.306	26.689	26.693	1.894	1.617	17.8043	0.9947	
4	11	1	25.357	24.041	24.075	0.842	1.317	13.9393	0.9959	
4	12	1	19.744	18.788	-18.750	-1.497	0.956	9.6372	0.9977	
4	13	1	1.201 *	0.906	-0.822	-0.379	0.296	0.4926	1.0000	* **
4	14	1	6.159	5.411	5.314	1.020	0.749	4.9149	0.9998	
4	0	2	10.871	11.517	-11.383	-1.782	-0.646	-9.9974	0.9992	
4	1	2	35.815	35.412	-35.547	-0.891	0.403	7.1035	0.9918	
4	2	2	45.999	45.345	45.624	2.400	0.654	11.1220	0.9851	
4	3	2	14.819	15.022	-15.028	0.387	-0.203	-3.1100	0.9986	
4	4	2	15.893	16.089	-16.045	-1.353	-0.196	-2.8765	0.9984	
4	5	2	7.097	7.201	-7.184	-0.512	-0.104	-1.1197	0.9997	
4	6	2	44.432	45.569	45.852	1.256	-1.137	-15.9689	0.9870	
4	7	2	8.668	8.874	8.868	0.386	-0.206	-2.1320	0.9994	
4	8	2	17.935	18.174	18.192	0.103	-0.239	-2.8151	0.9979	
4	9	2	10.573	10.164	10.165	0.207	0.409	4.1788	0.9993	
4	10	2	6.995	6.803	6.802	-0.150	0.192	1.5801	0.9997	
4	11	2	3.698	3.884	3.878	-0.214	-0.186	-0.9162	0.9999	
4	12	2	33.964	32.716	32.799	1.468	1.248	13.1659	0.9929	
4	13	2	5.909	5.974	-5.971	0.220	-0.065	-0.4234	0.9998	
4	14	2	7.522	6.845	-6.736	-1.221	0.676	4.8596	0.9998	
4	1	3	14.543	14.730	-14.739	-0.070	-0.187	-2.9351	0.9988	
4	2	3	24.737	24.888	-24.916	-0.872	-0.151	-2.4600	0.9966	
4	3	3	6.315	6.722	6.716	-0.304	-0.407	-4.6668	0.9998	
4	4	3	21.391	21.873	21.866	1.372	-0.483	-7.2840	0.9968	
4	5	3	24.465	24.408	24.435	0.776	0.058	0.8383	0.9967	
4	6	3	29.045	29.476	-29.490	-1.839	-0.431	-6.0204	0.9952	
4	7	3	4.681	4.542	-4.512	-0.521	0.140	1.0682	0.9999	
4	8	3	18.873	18.765	18.671	2.053	0.109	1.3183	0.9980	
4	9	3	4.211	4.082	4.041	0.583	0.129	0.8469	0.9999	
4	10	3	20.424	20.199	-20.143	-1.817	0.226	2.5242	0.9974	
4	11	3	21.860	22.117	-22.135	-0.816	-0.257	-2.7277	0.9970	
4	12	3	21.503	21.384	21.362	1.475	0.120	1.2384	0.9973	
4	13	3	3.634	3.773	-3.756	0.354	-0.138	-0.6499	0.9999	
4	0	4	65.452	64.400	65.038	2.414	1.052	17.0015	0.9791	
4	1	4	17.321	17.033	17.026	0.821	0.288	4.3567	0.9984	
4	2	4	8.393	8.258	-8.092	-1.658	0.135	1.7144	0.9996	
4	3	4	10.673	10.913	10.909	-0.372	-0.239	-3.1977	0.9994	
4	4	4	37.276	37.990	38.080	1.913	-0.714	-10.6129	0.9928	
4	5	4	18.952	19.195	19.205	0.531	-0.243	-3.3357	0.9982	
4	6	4	6.634	6.844	6.825	-0.527	-0.210	-2.0217	0.9997	
4	7	4	14.889	15.326	-15.330	-0.394	-0.437	-5.2724	0.9988	
4	8	4	10.462	10.289	10.280	0.503	0.174	1.8323	0.9994	
4	9	4	13.303	13.424	-13.429	-0.214	-0.121	-1.3067	0.9989	
4	10	4	7.402	7.651	7.621	0.686	-0.249	-2.1328	0.9997	
4	11	4	6.924	6.196	6.192	0.243	0.728	5.7976	0.9998	
4	12	4	1.300 *	1.392	-1.119	-0.828	-0.092	-0.1666	1.0000	* **
4	1	5	5.562	5.186	5.186	0.056	0.376	3.7552	0.9999	
4	2	5	6.652	5.679	5.625	0.783	0.973	10.4886	0.9998	
4	3	5	8.367	8.540	8.535	0.337	-0.173	-1.9897	0.9997	
4	4	5	6.262	5.873	-5.739	-1.249	0.389	3.9433	0.9998	
4	5	5	23.208	23.402	-23.421	-0.738	-0.194	-2.6073	0.9974	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	6	5	28.726	28.886	28.897	1.757	-0.160	-2.0993	0.9955
4	7	5	3.690	4.487	-4.462	0.468	-0.796	-4.6335	0.9999
4	8	5	27.748	28.070	-28.063	-1.969	-0.322	-3.8591	0.9957
4	9	5	5.941	6.386	6.366	-0.505	-0.445	-3.4668	0.9998
4	10	5	24.361	24.692	24.672	1.752	-0.331	-3.6804	0.9966
4	11	5	18.905	19.240	19.244	0.781	-0.334	-3.4712	0.9979
4	0	6	14.765	14.510	-14.431	-1.592	0.254	3.2360	0.9989
4	1	6	18.794	18.400	-18.399	-0.781	0.394	5.2195	0.9984
4	2	6	32.833	32.766	32.778	2.157	0.067	0.9160	0.9950
4	3	6	9.344	9.548	-9.544	0.338	-0.204	-2.2771	0.9996
4	4	6	7.997	7.529	-7.437	-1.180	0.468	4.7939	0.9997
4	5	6	9.845	10.062	-10.053	-0.474	-0.217	-2.3656	0.9995
4	6	6	24.805	25.494	25.508	1.106	-0.689	-8.4791	0.9970
4	7	6	9.404	9.425	9.420	0.362	-0.021	-0.2038	0.9996
4	8	6	13.332	13.590	13.596	0.106	-0.258	-2.7310	0.9991
4	9	6	8.586	8.702	8.701	0.198	-0.116	-1.0476	0.9996
4	10	6	8.759	8.385	8.385	-0.105	0.374	3.3258	0.9997
4	1	7	10.500	10.450	-10.452	-0.069	0.050	0.5489	0.9995
4	2	7	18.222	18.143	-18.141	-0.764	0.079	0.9631	0.9985
4	3	7	6.461	6.679	6.675	-0.249	-0.218	-1.8934	0.9998
4	4	7	16.430	16.396	16.363	1.193	0.034	0.3901	0.9988
4	5	7	15.256	15.295	15.288	0.682	-0.039	-0.4403	0.9989
4	6	7	18.733	18.940	-18.890	-1.580	-0.207	-2.3280	0.9983
4	7	7	5.273	5.164	-5.145	-0.446	0.109	0.7515	0.9999
4	8	7	10.953	10.592	10.446	1.774	0.360	3.4270	0.9995
4	0	8	32.835	32.501	32.511	2.013	0.334	3.9516	0.9956
4	1	8	14.883	14.841	14.831	0.712	0.042	0.4604	0.9991
4	2	8	4.369	3.514	-3.238	-1.366	0.855	5.4428	0.9999
4	3	8	6.399	6.873	6.867	-0.298	-0.474	-3.7868	0.9998
4	4	8	18.592	26.945	26.939	1.639	-8.353	-57.4359	0.9968
5	1	0	20.494	18.741	18.774	0.104	1.753	19.4997	0.9964
5	2	0	16.432	16.001	-16.015	-0.456	0.431	3.3220	0.9975
5	3	0	41.413	41.096	41.410	1.396	0.317	2.6073	0.9837
5	4	0	17.079	17.050	17.066	0.495	0.029	0.2165	0.9973
5	5	0	27.050	25.066	-25.097	-1.463	1.984	14.7280	0.9942
5	6	0	2.190	0.698	0.178	-0.674	1.493	3.0553	1.0000
5	7	0	26.244	24.168	24.143	2.036	2.076	15.1541	0.9950
5	8	0	13.029	11.113	11.078	0.942	1.916	12.1825	0.9990
5	9	0	6.967	6.694	6.536	-1.450	0.274	1.3430	0.9997
5	10	0	5.863	4.697	-4.646	-0.694	1.166	4.9606	0.9998
5	11	0	47.829	44.273	44.508	2.093	3.556	24.9220	0.9873
5	12	0	5.111	4.417	4.381	0.568	0.693	2.6792	0.9999
5	0	1	3.170	1.846	-1.703	0.713	1.324	11.1164	1.0000
5	1	1	39.654	39.830	-39.975	-2.122	-0.176	-2.7599	0.9900
5	2	1	18.458	18.733	-18.736	-0.896	-0.275	-3.9110	0.9974
5	3	1	4.102	4.528	4.266	1.521	-0.427	-3.2741	0.9998
5	4	1	14.039	14.195	14.187	0.760	-0.157	-1.8746	0.9984
5	5	1	28.544	28.672	-28.740	-1.287	-0.128	-1.5803	0.9933
5	6	1	1.691	0.305	-0.133	-0.274	1.387	4.0999	1.0000
5	7	1	17.701	17.247	17.254	0.691	0.454	4.8769	0.9976
5	8	1	5.589	5.685	5.684	0.159	-0.096	-0.6595	0.9998
5	9	1	15.221	14.282	14.289	0.324	0.939	9.0273	0.9986
5	10	1	3.416	2.929	2.928	0.058	0.488	2.0519	0.9999

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
5	11	1	9.714		9.247	-9.217	-0.772	0.468	3.5991	0.9995	
5	12	1	6.226		5.180	-5.157	-0.494	1.046	6.4749	0.9998	
5	1	2	6.938		7.001	6.982	0.529	-0.063	-0.7933	0.9997	
5	2	2	3.335		1.084	-1.006	0.405	2.251	17.7853	1.0000	
5	3	2	16.698		17.291	17.292	-0.656	-0.593	-8.3475	0.9985	
5	4	2	3.011		3.311	-3.280	-0.447	-0.299	-1.8195	0.9999	
5	5	2	50.169		50.552	50.961	2.070	-0.382	-5.1407	0.9824	
5	6	2	4.719		4.488	4.436	0.681	0.231	1.7607	0.9999	
5	7	2	8.124		8.168	-8.044	-1.427	-0.045	-0.4253	0.9996	
5	8	2	24.115		24.312	-24.342	-0.972	-0.197	-2.2419	0.9959	
5	9	2	32.644		33.352	33.416	2.077	-0.707	-7.7264	0.9923	
5	10	2	11.485		11.402	11.385	0.711	0.083	0.7633	0.9992	
5	11	2	22.888		21.611	-21.592	-1.496	1.277	12.5590	0.9970	
5	12	2	2.155		2.093	2.024	-0.531	0.062	0.1679	1.0000	
5	0	3	5.761		6.053	-6.012	-0.708	-0.292	-3.2072	0.9998	
5	1	3	43.782		44.078	44.239	2.087	-0.296	-4.5469	0.9905	
5	2	3	20.126		20.513	20.515	0.887	-0.387	-5.6515	0.9980	
5	3	3	2.484		2.828	-2.416	-1.469	-0.344	-1.8904	1.0000	
5	4	3	7.978		7.840	-7.808	-0.718	0.138	1.5391	0.9997	
5	5	3	18.108		18.038	18.014	1.228	0.070	0.9099	0.9980	
5	6	3	6.002		6.197	-6.192	0.249	-0.195	-1.7480	0.9998	
5	7	3	10.450		10.248	-10.230	-0.648	0.202	2.1566	0.9995	
5	8	3	4.988		4.015	-4.012	-0.145	0.973	6.7669	0.9999	
5	9	3	9.921		9.956	-9.955	-0.298	-0.035	-0.3226	0.9995	
5	10	3	1.378	*	1.999	1.999	-0.033	-0.621	-1.2308	1.0000	* **
5	11	3	2.981		2.551	2.444	0.733	0.430	1.6671	1.0000	
5	1	4	17.182		17.374	17.386	0.114	-0.191	-2.6456	0.9986	
5	2	4	10.512		10.214	-10.208	-0.423	0.298	3.7354	0.9995	
5	3	4	28.771		29.632	29.669	1.310	-0.861	-11.9804	0.9956	
5	4	4	10.894		11.591	11.586	0.457	-0.697	-8.3372	0.9993	
5	5	4	20.256		20.211	-20.184	-1.373	0.045	0.5786	0.9981	
5	6	4	1.327	*	0.909	-0.648	-0.638	0.418	1.1000	1.0000	* **
5	7	4	22.020		22.900	22.853	1.933	-0.880	-10.6106	0.9970	
5	8	4	12.463		11.988	11.959	0.901	0.475	5.0701	0.9993	
5	9	4	2.028		2.671	2.293	-1.371	-0.644	-1.9890	1.0000	
5	10	4	5.983		5.725	-5.688	-0.658	0.258	1.8210	0.9998	
5	11	4	38.478		38.799	38.923	1.983	-0.321	-3.3192	0.9911	
5	0	5	5.918		6.249	-6.217	0.637	-0.330	-2.0970	0.9998	
5	1	5	25.205		24.850	-24.810	-1.927	0.355	4.8240	0.9973	
5	2	5	11.762		11.813	-11.789	-0.809	-0.051	-0.6183	0.9994	
5	3	5	4.763		4.593	4.376	1.393	0.171	1.3998	0.9999	
5	4	5	14.278		14.322	14.311	0.715	-0.043	-0.5255	0.9990	
5	5	5	26.929		27.722	-27.749	-1.195	-0.793	-9.8142	0.9962	
5	6	5	4.303		4.649	-4.642	-0.258	-0.347	-2.4034	0.9999	
5	7	5	16.875		17.279	17.280	0.655	-0.404	-4.5901	0.9984	
5	8	5	4.963		5.376	5.374	0.154	-0.412	-2.8732	0.9999	
5	9	5	12.930		13.614	13.617	0.316	-0.684	-6.7932	0.9990	
5	1	6	7.098		7.661	7.647	0.488	-0.563	-5.3997	0.9997	
5	2	6	4.180		3.609	3.589	0.381	0.571	4.0857	0.9999	
5	3	6	5.759		5.751	5.721	-0.592	0.008	0.0668	0.9999	
5	4	6	6.245		6.322	-6.310	-0.407	-0.078	-0.6695	0.9998	
5	5	6	37.085		37.914	37.993	1.865	-0.829	-10.0886	0.9935	
5	6	6	2.835		2.352	2.274	0.600	0.483	2.3458	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
5	7	6	3.951	3.471	-3.242	-1.239	0.480	2.8716	0.9999	
5	0	7	6.635	6.599	-6.572	-0.608	0.036	0.3165	0.9998	
5	1	7	31.976	32.112	32.131	1.816	-0.136	-1.6375	0.9957	
5	2	7	14.862	14.907	14.894	0.778	-0.045	-0.5019	0.9989	
5	3	7	3.048	2.132	-1.722	-1.257	0.916	4.7169	1.0000	
5	4	7	3.962	3.488	-3.433	-0.613	0.474	2.9366	0.9999	
6	0	0	4.788	4.581	4.181	1.873	0.208	1.2376	0.9999	
6	1	0	26.053	24.249	24.291	1.028	1.804	12.6335	0.9948	
6	2	0	19.561	18.849	-18.817	-1.510	0.711	4.9290	0.9971	
6	3	0	6.976	6.734	-6.689	-0.783	0.242	1.1618	0.9996	
6	4	0	50.248	48.381	48.827	1.847	1.867	13.2404	0.9804	
6	5	0	4.754	4.695	-4.660	0.577	0.058	0.1964	0.9998	
6	6	0	21.663	20.174	20.207	-0.252	1.489	9.2758	0.9966	
6	7	0	5.363	4.024	-4.011	-0.335	1.339	4.5379	0.9999	
6	8	0	23.136	21.417	21.450	0.523	1.719	10.4971	0.9964	
6	9	0	2.771	1.822	-1.821	-0.061	0.950	1.9165	1.0000	
6	10	0	9.527	8.878	8.864	0.550	0.649	3.1748	0.9994	
6	1	1	8.431	8.657	8.658	-0.099	-0.226	-2.5603	0.9997	
6	2	1	28.646	28.670	28.716	0.898	-0.024	-0.3123	0.9958	
6	3	1	6.063	5.711	5.691	0.484	0.352	2.8886	0.9998	
6	4	1	3.159	3.249	-3.081	-1.032	-0.091	-0.4257	0.9999	
6	5	1	14.307	13.725	-13.711	-0.792	0.583	5.8681	0.9986	
6	6	1	10.337	9.981	9.872	1.496	0.355	3.1635	0.9992	
6	7	1	6.671	6.326	6.271	0.836	0.345	2.3613	0.9997	
6	8	1	41.152	38.966	-39.137	-1.953	2.186	21.4938	0.9888	
6	9	1	14.526	13.727	-13.707	-0.887	0.799	6.7189	0.9987	
6	10	1	8.187	7.413	7.271	1.451	0.773	4.9996	0.9996	
6	0	2	13.645	13.925	13.876	-1.238	-0.280	-3.6890	0.9991	
6	1	2	6.558	5.990	-5.914	-0.956	0.568	5.9078	0.9998	
6	2	2	49.921	51.341	51.660	2.145	-1.420	-19.2245	0.9860	
6	3	2	8.988	9.473	9.443	0.782	-0.485	-5.2068	0.9995	
6	4	2	12.633	12.379	-12.330	-1.165	0.254	2.8186	0.9990	
6	5	2	12.865	13.702	-13.696	-0.629	-0.837	-8.9004	0.9988	
6	6	2	4.180	4.210	-4.128	0.827	-0.029	-0.1705	0.9999	
6	7	2	14.864	15.480	15.486	0.375	-0.616	-6.1150	0.9987	
6	8	2	3.070	2.929	2.928	0.081	0.141	0.5701	0.9999	
6	9	2	8.888	8.838	8.840	0.091	0.050	0.3895	0.9995	
6	10	2	17.987	18.146	18.166	0.050	-0.159	-1.4262	0.9978	
6	1	3	2.994	2.726	-2.724	0.120	0.268	1.6105	1.0000	
6	2	3	21.598	21.696	-21.702	-0.857	-0.098	-1.2760	0.9979	
6	3	3	12.992	13.807	-13.804	-0.494	-0.815	-9.5308	0.9991	
6	4	3	1.388 *	1.154	-0.591	0.991	0.234	0.6268	1.0000	* **
6	5	3	15.554	15.454	15.443	0.785	0.100	1.1419	0.9989	
6	6	3	10.076	10.389	-10.290	-1.452	-0.313	-3.1058	0.9994	
6	7	3	2.145	0.838	0.298	-0.784	1.306	4.6038	1.0000	
6	8	3	39.877	40.827	40.964	1.921	-0.950	-10.2851	0.9911	
6	9	3	6.714	6.504	6.450	0.842	0.210	1.4642	0.9998	
6	0	4	7.425	5.934	5.662	1.776	1.492	15.2459	0.9998	
6	1	4	17.228	17.406	17.392	0.958	-0.178	-2.2308	0.9986	
6	2	4	17.438	17.408	-17.361	-1.423	0.030	0.3751	0.9986	
6	3	4	6.230	6.361	-6.319	-0.739	-0.132	-1.1810	0.9998	
6	4	4	38.502	40.038	40.160	1.745	-1.536	-19.0650	0.9921	
6	5	4	1.652	0.801	-0.576	0.557	0.851	2.4990	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
6	6	4	17.655	18.834	18.851	-0.221	-1.179	-13.1641	0.9981	
6	7	4	5.648	5.818	-5.810	-0.325	-0.171	-1.2511	0.9998	
6	8	4	16.884	18.248	18.258	0.498	-1.364	-13.8396	0.9981	
6	1	5	10.468	10.512	10.514	-0.071	-0.044	-0.4889	0.9995	
6	2	5	25.363	25.799	25.823	0.842	-0.436	-5.3242	0.9971	
6	3	5	1.684	1.306	-1.233	0.428	0.378	1.1728	1.0000	
6	4	5	5.290	5.447	-5.364	-0.947	-0.157	-1.2144	0.9999	
6	5	5	9.112	9.201	-9.175	-0.714	-0.089	-0.8457	0.9996	
6	6	5	7.706	7.657	7.534	1.370	0.049	0.4338	0.9997	
6	0	6	11.523	12.619	12.578	-1.069	-1.096	-11.2347	0.9993	
6	1	6	9.643	9.525	-9.487	-0.871	0.118	1.1710	0.9996	
6	2	6	36.072	36.915	36.983	1.917	-0.842	-9.9539	0.9936	
6	3	6	6.721	6.675	6.640	0.691	0.046	0.3860	0.9998	
7	1	0	30.497	28.341	28.435	0.240	2.156	12.9093	0.9933	
7	2	0	3.851	4.536	-4.525	-0.317	-0.686	-1.8678	0.9998	
7	3	0	12.929	12.036	11.993	1.097	0.893	4.8789	0.9989	
7	4	0	1.827 *	0.700	0.172	0.679	1.127	1.4525	1.0000	* **
7	5	0	13.341	11.208	-11.153	-1.164	2.134	11.0591	0.9990	
7	6	0	15.770	13.790	-13.772	-0.903	1.980	10.2353	0.9984	
7	7	0	27.692	24.674	24.684	1.652	3.018	16.3209	0.9948	
7	0	1	14.745	14.757	14.723	1.101	-0.012	-0.1442	0.9990	
7	1	1	25.070	25.727	-25.714	-1.720	-0.656	-7.7830	0.9965	
7	2	1	9.947	9.759	-9.715	-0.944	0.188	1.7770	0.9995	
7	3	1	7.951	7.322	7.252	1.156	0.629	5.0625	0.9996	
7	4	1	10.306	9.920	9.894	0.750	0.386	3.2109	0.9994	
7	5	1	8.181	7.310	-7.244	-0.989	0.871	6.3315	0.9996	
7	6	1	4.070	4.114	-4.081	-0.525	-0.044	-0.1875	0.9999	
7	7	1	14.896	14.145	14.144	0.595	0.750	6.0581	0.9984	
7	1	2	6.191	6.377	6.364	0.419	-0.186	-1.6674	0.9998	
7	2	2	10.052	10.381	10.378	0.335	-0.329	-3.3666	0.9994	
7	3	2	7.297	7.363	-7.344	-0.537	-0.066	-0.5581	0.9997	
7	4	2	5.344	4.844	-4.796	-0.684	0.500	3.3439	0.9999	
7	5	2	35.913	36.957	37.047	1.765	-1.044	-10.9413	0.9929	
7	6	2	12.211	11.813	11.785	0.887	0.398	3.6268	0.9991	
7	0	3	10.951	10.528	-10.478	-1.051	0.423	4.4895	0.9995	
7	1	3	17.429	16.889	16.819	1.645	0.540	6.2133	0.9987	
7	2	3	8.501	8.246	8.196	0.920	0.255	2.4218	0.9997	
7	3	3	8.026	8.171	-8.095	-1.122	-0.144	-1.3127	0.9997	
7	4	3	10.656	10.953	-10.932	-0.727	-0.297	-2.8736	0.9994	
7	5	3	14.242	14.623	14.598	0.994	-0.381	-3.8171	0.9988	
7	1	4	21.648	22.398	22.421	0.228	-0.750	-8.6226	0.9978	
7	2	4	5.050	5.323	-5.315	-0.302	-0.273	-1.9230	0.9999	

IHC209I IBCOM - PROGRAM INTERRUPT (P) - DIVIDE CHECK OLD PSW IS 078D000F42093046 . REGISTER CONTAINED 0000000052160000

TRACEBACK ROUTINE	CALLED FROM ISN	REG. 14	REG. 15	REG. 0	REG. 1
TESTS	0015	4209281A	00092E88	00000001	0009260C
INPUT	0122	420A083E	00092448	00000001	0009DB00
RFINE	0007	4208615E	0009D510	0087D0D8	00000000
MAIN		0000AF58	00085F80	0087D0D8	00084FF8

ENTRY POINT= 00085F80

STANDARD FIXUP TAKEN , EXECUTION CONTINUING

RESULTS OF STRUCTURE FACTOR CALCULATIONS

RFINE F051TE49 FINAL CYCLE

	NUMERATOR	DENOMINATOR	NUMBER	R
ALL REFLECTIONS				
WEIGHTED R	76529.69	98295360.00	731	0.028
UNWEIGHTED R	387.10	13372.56	731	0.029
RANGES OF F(OBS)				
	12357.42	54996976.00	409	0.015
	13784.93	25548720.00	190	0.023
	12102.32	9412686.00	70	0.036
	26494.09	5109745.00	38	0.072
	2570.74	1210202.00	9	0.046
	3968.74	941268.69	7	0.065
	56.85	134466.94	1	0.021
	5199.80	941268.69	7	0.074
RANGES OF (SIN(THETA)/LAMBDA)**2				
	43109.16	5109745.00	38	0.092
	7815.09	7799080.00	58	0.032
	4999.67	10353953.00	77	0.022
	3864.24	12102026.00	90	0.018
	2769.07	13043292.00	97	0.015
	2932.21	15463699.00	115	0.014
	4263.11	16404966.00	122	0.016
	6783.21	18018560.00	134	0.019
UNREJECTED REFLECTIONS				
WEIGHTED R	76498.38	98295360.00	710	0.028
UNWEIGHTED R	374.43	13346.25	710	0.028
RANGES OF F(OBS)				
	12326.01	53716336.00	388	0.015
	13784.93	26304384.00	190	0.023
	12102.32	9691087.00	70	0.035
	26494.09	5260878.00	38	0.071
	2570.74	1245997.00	9	0.045
	3968.74	969108.88	7	0.064
	56.85	138444.13	1	0.020
	5199.80	969108.88	7	0.073
RANGES OF (SIN(THETA)/LAMBDA)**2				
	43109.16	5260878.00	38	0.091
	7813.09	7891316.00	57	0.031
	4992.81	10383311.00	75	0.022
	3859.81	12183083.00	88	0.018
	2769.07	13429081.00	97	0.014
	2924.28	14951968.00	108	0.014
	4258.88	16336411.00	118	0.016
	6777.21	17859280.00	129	0.019

SUM FCAL 13263.44
STANDARD DEV OF UNIT WEIGHT OBS 10.69

RFINE F051TE49 FINAL CYCLE

ATOM	PARAMETER	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR	
ESTIMATED STD. DEV. FOR OBS. OF UNIT WEIGHT		10.69					
EXTINCTION CORRECTION ISOTROPIC							
	R-STAR	0.8804E-01	-.5600E-05	0.8803E-01	0.3932E-02	-0.00	1
	SCALE FACTOR 1	8.5120		8.5120			
ATOM 1 M1	EQUIPOINT FRACTION = 0.500						
	OCCUPANCY SPECIES 1	0.92050	0.00000	0.92050	0.00487	0.00	2
	OCCUPANCY SPECIES 2	0.07950		0.07950			
	TOTAL OCCUPANCY (FIXED) =	1.00000					
	X	0.0		0.0			
	Y	0.0		0.0			
	Z	0.0		0.0			
	BETA11	0.0030700	-0.0000035	0.0030665	0.0003839	-0.01	3
	BETA22	0.0013500	-0.0000001	0.0013499	0.0000848	-0.00	4
	BETA33	0.0024700	0.0000001	0.0024701	0.0002282	0.00	5
	BETA12	-0.0000700	0.0000040	-0.0000660	0.0001555	0.03	6
	BETA13	-0.0004600	0.0000013	-0.0004587	0.0002153	0.01	7
	BETA23	-0.0003400	-0.0000030	-0.0003430	0.0000902	-0.03	8
ATOM 2 M2	EQUIPOINT FRACTION = 0.500						
	OCCUPANCY SPECIES 1	0.10950		0.10950			
	OCCUPANCY SPECIES 2	0.89050		0.89050			
	TOTAL OCCUPANCY (FIXED) =	1.00000					
	X	0.9870400	0.0000003	0.9870402	0.0001115	0.00	9
	Y	0.2790400	-0.0000027	0.2790373	0.0000493	-0.05	10
	Z	0.2500000		0.2500000			
	BETA11	0.0061200	-0.0000044	0.0061156	0.0001754	-0.03	11
	BETA22	0.0011600	0.0000045	0.0011645	0.0000354	0.13	12
	BETA33	0.0036600	-0.0000006	0.0036594	0.0000934	-0.01	13
	BETA12	0.0002400	-0.0000031	0.0002369	0.0000818	-0.04	14
	BETA13	0.0		0.0			
	BETA23	0.0		0.0			
ATOM 3 S1	EQUIPOINT FRACTION = 0.500						
	OCCUPANCY SPECIES 3	1.00000		1.00000			
	X	0.4226200	0.0000036	0.4226235	0.0001781	0.02	15
	Y	0.0909899	0.0000005	0.0909904	0.0000886	0.01	16
	Z	0.2500000		0.2500000			
	BETA11	0.0031200	-0.0000044	0.0031156	0.0002885	-0.02	17
	BETA22	0.0009600	0.0000029	0.0009629	0.0000629	0.05	18
	BETA33	0.0025200	-0.0000049	0.0025151	0.0001596	-0.03	19
	BETA12	0.0000400	-0.0000013	0.0000387	0.0001211	-0.01	20
	BETA13	0.0		0.0			
	BETA23	0.0		0.0			
ATOM 4 O1	EQUIPOINT FRACTION = 0.500						
	OCCUPANCY SPECIES 4	1.00000		1.00000			
	X	0.7585000	0.0000032	0.7585031	0.0004550	0.01	21
	Y	0.0867100	-0.0000010	0.0867089	0.0002286	-0.00	22
	Z	0.2500000		0.2500000			
	BETA11	0.0022000	0.0000023	0.0022023	0.0007394	0.00	23
	BETA22	0.0016900	0.0000017	0.0016917	0.0001866	0.01	24
	BETA33	0.0036500	0.0000047	0.0036547	0.0004286	0.01	25
	BETA12	-0.0001600	0.0000015	-0.0001585	0.0003473	0.00	26
	BETA13	0.0		0.0			
	BETA23	0.0		0.0			

ATOM 5	O2	EQUIPOINT FRACTION = 0.500						
		OCCUPANCY SPECIES 4	1.00000		1.00000			
		X	0.2300500	0.0000021	0.2300521	0.0004683	0.00	27
		Y	0.4488900	0.0000021	0.4488921	0.0002144	0.01	28
		Z	0.2500000		0.2500000			
		BETA11	0.0040200	-0.0000010	0.0040190	0.0007768	-0.00	29
		BETA22	0.0011200	-0.0000042	0.0011158	0.0001712	-0.02	30
		BETA33	0.0037800	-0.0000045	0.0037755	0.0004259	-0.01	31
		BETA12	-0.0004800	-0.0000027	-0.0004827	0.0003337	-0.01	32
		BETA13	0.0		0.0			
		BETA23	0.0		0.0			
ATOM 6	O3	EQUIPOINT FRACTION = 1.000						
		OCCUPANCY SPECIES 4	1.00000		1.00000			
		X	0.2781799	0.0000040	0.2781839	0.0003285	0.01	33
		Y	0.1589600	-0.0000008	0.1589592	0.0001554	-0.01	34
		Z	0.0374200	0.0000040	0.0374240	0.0002202	0.02	35
		BETA11	0.0039400	-0.0000012	0.0039388	0.0005576	-0.00	36
		BETA22	0.0013400	-0.0000037	0.0013363	0.0001209	-0.03	37
		BETA33	0.0036200	0.0000009	0.0036209	0.0003033	0.00	38
		BETA12	-0.0000200	0.0000032	-0.0000168	0.0002288	0.01	39
		BETA13	-0.0000400	0.0000005	-0.0000395	0.0003346	0.00	40
		BETA23	0.0003700	-0.0000037	0.0003663	0.0001641	-0.02	41

MAXIMUM SHIFT/ERROR = 0.13

AVERAGE SHIFT/ERROR = 0.02

RFINE F051TE49 FINAL CYCLE

CORRELATION MATRIX

ROW 1

1 1.0000	2 -0.3154	3 0.1394	4 0.0766	5 0.1592	6 -0.0015	7 0.0016	8 -0.0038	9 0.0261	10 -0.0081
11 -0.0590	12 -0.1260	13 -0.0520	14 -0.0091	15 0.0410	16 -0.0255	17 0.0005	18 -0.0603	19 -0.0422	20 -0.0251
21 -0.0340	22 0.0224	23 0.0019	24 -0.1086	25 -0.0123	26 -0.0022	27 0.0251	28 -0.0794	29 -0.0315	30 -0.0187
31 0.0045	32 0.0017	33 -0.0092	34 0.0231	35 -0.0382	36 -0.0398	37 -0.1061	38 -0.0076	39 0.0204	40 0.0035
41 -0.0277									

ROW 2

2 1.0000	3 -0.5401	4 -0.5066	5 -0.5502	6 0.0003	7 0.0038	8 0.0097	9 -0.0168	10 -0.0083	11 0.0259
12 0.0612	13 0.0292	14 0.0026	15 -0.0030	16 0.0233	17 0.0160	18 0.0268	19 0.0220	20 -0.0023	21 0.0293
22 0.0391	23 0.0151	24 0.0456	25 0.0184	26 -0.0047	27 -0.0062	28 0.0164	29 0.0318	30 -0.0005	31 0.0263
32 0.0137	33 0.0370	34 -0.0151	35 0.0717	36 0.0520	37 0.0278	38 0.0282	39 -0.0077	40 -0.0065	41 0.0291

ROW 3

3 1.0000	4 0.1539	5 0.1068	6 -0.0026	7 -0.0134	8 0.0025	9 0.0193	10 -0.0013	11 -0.0410	12 -0.0219
13 0.0077	14 -0.0030	15 -0.0105	16 -0.0157	17 -0.0806	18 -0.0035	19 -0.0052	20 0.0056	21 -0.0372	22 -0.0209
23 -0.0404	24 -0.0113	25 -0.0209	26 -0.0099	27 0.0224	28 -0.0185	29 -0.0319	30 0.0061	31 -0.0280	32 -0.0164
33 -0.0164	34 -0.0077	35 -0.0333	36 -0.0545	37 -0.0106	38 -0.0080	39 -0.0136	40 0.0034	41 0.0084	

ROW 4

4 1.0000	5 0.0865	6 -0.0035	7 0.0010	8 -0.0249	9 0.0079	10 0.0190	11 -0.0006	12 -0.1551	13 0.0301
14 0.0007	15 -0.0082	16 -0.0199	17 0.0018	18 -0.0036	19 -0.0068	20 0.0087	21 -0.0079	22 -0.0542	23 0.0050
24 -0.0195	25 -0.0194	26 -0.0130	27 0.0045	28 -0.0106	29 -0.0090	30 -0.0007	31 -0.0236	32 -0.0141	33 -0.0348
34 0.0206	35 -0.0267	36 -0.0244	37 -0.0054	38 -0.0205	39 0.0018	40 0.0069	41 -0.0262		

ROW 5

5 1.0000	6 0.0034	7 -0.0166	8 -0.0270	9 0.0143	10 0.0124	11 0.0071	12 0.0097	13 -0.1510	14 -0.0025
15 0.0046	16 -0.0064	17 -0.0046	18 -0.0119	19 -0.0050	20 -0.0025	21 -0.0183	22 -0.0125	23 -0.0178	24 -0.0353
25 0.0220	26 0.0175	27 -0.0062	28 -0.0134	29 -0.0335	30 -0.0059	31 0.0252	32 -0.0117	33 -0.0124	34 0.0069
35 -0.0548	36 -0.0203	37 -0.0218	38 0.0050	39 0.0075	40 0.0003	41 -0.0537			

ROW 6

6 1.0000	7 -0.0170	8 -0.0105	9 -0.0203	10 0.0082	11 -0.0160	12 -0.0025	13 0.0036	14 -0.0342	15 -0.0087
16 0.0456	17 0.0258	18 0.0249	19 -0.0119	20 -0.0165	21 -0.0066	22 -0.0099	23 -0.0312	24 -0.0301	25 0.0248
26 0.0315	27 -0.0254	28 -0.0008	29 -0.0420	30 0.0037	31 0.0120	32 -0.0351	33 0.0356	34 0.0043	35 -0.0154
36 -0.0033	37 -0.0479	38 0.0081	39 -0.0369	40 -0.0151	41 0.0010				

ROW 7

7 1.0000	8 -0.0024	9 0.0505	10 -0.0044	11 0.0192	12 -0.0059	13 0.0168	14 0.0222	15 0.0321	16 0.0010
17 -0.0259	18 0.0124	19 -0.0347	20 -0.0005	21 0.0229	22 0.0048	23 0.0029	24 -0.0015	25 -0.0034	26 -0.0013
27 -0.0251	28 0.0050	29 -0.0109	30 0.0010	31 -0.0038	32 0.0007	33 0.0054	34 0.0211	35 -0.0073	36 -0.0244
37 -0.0045	38 0.0270	39 -0.0345	40 -0.0057	41 0.0159					

ROW 8

8 1.0000	9 0.0014	10 0.0044	11 -0.0057	12 -0.0154	13 0.0043	14 0.0013	15 0.0019	16 0.0065	17 -0.0120
18 0.0059	19 0.0154	20 -0.0043	21 -0.0043	22 0.0073	23 -0.0098	24 0.0035	25 -0.0117	26 0.0134	27 0.0116
28 -0.0011	29 0.0224	30 0.0039	31 -0.0083	32 0.0165	33 0.0015	34 -0.0228	35 0.0040	36 0.0046	37 -0.0131
38 -0.0219	39 -0.0326	40 -0.0007	41 0.0107						

ROW 9

9 1.0000	10 0.0048	11 0.0502	12 0.0189	13 -0.0041	14 0.0247	15 0.0408	16 0.0360	17 -0.0193	18 -0.0466
19 0.0054	20 -0.0090	21 -0.0093	22 0.0092	23 0.0744	24 -0.0057	25 -0.0282	26 0.0121	27 0.0418	28 0.0106
29 -0.0744	30 0.0077	31 0.0347	32 -0.0105	33 0.0182	34 0.0088	35 -0.0222	36 -0.0291	37 -0.0078	38 0.0138
39 -0.0077	40 -0.0051	41 0.0035							

ROW 10

10 1.0000	11 -0.0072	12 0.0116	13 0.0030	14 -0.0430	15 -0.0158	16 0.0339	17 0.0093	18 -0.0188	19 -0.0065
20 0.0337	21 -0.0192	22 -0.0146	23 0.0058	24 -0.0178	25 0.0072	26 -0.0100	27 -0.0228	28 0.0050	29 -0.0045
30 -0.0446	31 -0.0014	32 -0.0294	33 0.0092	34 0.0264	35 0.0099	36 -0.0040	37 0.0258	38 -0.0037	39 -0.0007
40 0.0069	41 -0.0291								

```
ROW  11
11  1.0000   12 -0.1682   13 -0.2630   14  0.0229   15  0.0309   16 -0.0007   17 -0.1100   18  0.0185   19  0.0495   20 -0.0
21  0.0532   22 -0.0089   23  0.0064   24 -0.0009   25  0.0059   26  0.0126   27 -0.0150   28 -0.0017   29 -0.0487   30  0.0
31  0.0196   32  0.0177   33 -0.0226   34  0.0090   35 -0.0134   36 -0.0625   37  0.0045   38  0.0015   39  0.0037   40  0.0
41 -0.0139

ROW  12
12  1.0000   13 -0.2521   14  0.0088   15 -0.0070   16  0.0278   17  0.0180   18 -0.1199   19  0.0549   20  0.0125   21 -0.0
22  0.0048   23 -0.0042   24  0.0129   25  0.0119   26  0.0143   27 -0.0048   28  0.0390   29  0.0025   30 -0.0284   31  0.0
32 -0.0192   33  0.0133   34 -0.0175   35 -0.0005   36  0.0052   37  0.0236   38 -0.0012   39 -0.0105   40 -0.0116   41  0.00

ROW  13
13  1.0000   14 -0.0007   15  0.0225   16 -0.0013   17  0.0446   18  0.0318   19 -0.1173   20 -0.0052   21  0.0013   22
23  0.0095   24  0.0157   25 -0.0308   26 -0.0054   27  0.0041   28  0.0072   29  0.0251   30  0.0154   31 -0.0540   32
33  0.0094   34 -0.0156   35  0.0497   36  0.0041   37  0.0042   38  0.0034   39 -0.0061   40  0.0217   41  0.0472

ROW  14
14  1.0000   15 -0.0042   16 -0.0585   17 -0.0179   18  0.0125   19 -0.0037   20  0.0121   21 -0.0017   22 -0.0364   23 -0.
24  0.0022   25  0.0051   26 -0.0056   27  0.0226   28  0.0311   29  0.0154   30  0.0079   31  0.0088   32 -0.0004   33 -0.
34 -0.0085   35  0.0041   36 -0.0093   37 -0.0040   38  0.0043   39 -0.0226   40  0.0218   41 -0.0094

ROW  15
15  1.0000   16  0.0053   17 -0.0694   18  0.0120   19  0.0113   20 -0.0329   21  0.0342   22  0.0028   23  0.0922   24 -0.0
25 -0.0203   26  0.0060   27 -0.0001   28  0.0082   29  0.0077   30  0.0050   31 -0.0218   32 -0.0230   33  0.0109   34  0.00
35  0.0232   36  0.0229   37 -0.0052   38 -0.0173   39  0.0264   40 -0.0181   41  0.0060

ROW  16
16  1.0000   17  0.0153   18  0.0018   19 -0.0059   20 -0.0315   21 -0.0017   22 -0.1912   23  0.0219   24 -0.0674   25  0.0
26  0.0310   27  0.0046   28  0.0033   29 -0.0241   30 -0.0319   31  0.0151   32  0.0221   33  0.0267   34  0.0149   35  0.0
36 -0.0082   37  0.0136   38  0.0019   39 -0.0316   40  0.0081   41  0.0092

ROW  17
17  1.0000   18 -0.2000   19 -0.2666   20 -0.0004   21 -0.0535   22 -0.0058   23 -0.1323   24  0.0617   25  0.0686   26 -0.0
27  0.0268   28  0.0152   29 -0.0241   30 -0.0099   31  0.0202   32  0.0109   33  0.0300   34 -0.0058   35  0.0016   36  0.0
37  0.0083   38  0.0000   39  0.0038   40 -0.0144   41  0.0031

ROW  18
18  1.0000   19 -0.2510   20  0.0059   21  0.0154   22  0.0403   23  0.0566   24 -0.2530   25  0.0414   26  0.0020   27 -0.02
28 -0.0015   29 -0.0031   30 -0.0106   31  0.0134   32  0.0213   33 -0.0003   34  0.0057   35 -0.0091   36  0.0065   37 -0.07
38  0.0368   39  0.0108   40  0.0064   41 -0.0003

ROW  19
19  1.0000   20 -0.0087   21  0.0166   22  0.0038   23  0.0717   24  0.0395   25 -0.1760   26  0.0067   27  0.0012   28 -0.02
29  0.0187   30  0.0149   31 -0.0513   32 -0.0151   33 -0.0112   34 -0.0087   35  0.0363   36  0.0024   37  0.0390   38 -0.09
39 -0.0032   40 -0.0305   41  0.0083

ROW  20
20  1.0000   21 -0.0011   22 -0.0081   23 -0.0005   24  0.0070   25  0.0110   26 -0.0426   27 -0.0068   28  0.0184   29 -0.0
30 -0.0073   31 -0.0005   32  0.0127   33 -0.0033   34  0.0049   35 -0.0160   36 -0.0114   37  0.0093   38  0.0037   39  0.00
40 -0.0124   41  0.0177

ROW  21
21  1.0000   22 -0.0090   23 -0.0113   24  0.0060   25 -0.0072   26 -0.0524   27 -0.0099   28 -0.0086   29 -0.0204   30  0.00
31 -0.0031   32  0.0341   33 -0.0087   34  0.0156   35  0.0019   36  0.0091   37  0.0075   38 -0.0056   39  0.0303   40 -0.30
41 -0.0165

ROW  22
22  1.0000   23  0.0140   24  0.0202   25 -0.0053   26  0.0056   27 -0.0086   28  0.0054   29  0.0052   30  0.0344   31  0.02
32 -0.0180   33  0.0045   34 -0.0160   35 -0.0349   36  0.0069   37 -0.0486   38  0.0117   39 -0.0025   40 -0.0092   41  0.03

ROW  23
23  1.0000   24 -0.1947   25 -0.2834   26 -0.0029   27  0.0065   28 -0.0061   29  0.0125   30  0.0327   31 -0.0371   32 -0.00
33 -0.0161   34  0.0036   35 -0.0010   36 -0.0139   37 -0.0045   38 -0.0159   39  0.0024   40 -0.0280   41  0.0004

ROW  24
24  1.0000   25 -0.2405   26 -0.0099   27  0.0039   28  0.0285   29  0.0101   30 -0.0043   31 -0.0043   32 -0.0019   33  0.00
34 -0.0080   35  0.0362   36 -0.0007   37  0.0825   38 -0.0145   39 -0.0075   40  0.0003   41  0.0090

ROW  25
25  1.0000   26  0.0029   27  0.0085   28  0.0221   29 -0.0365   30 -0.0022   31  0.0586   32  0.0054   33 -0.0086   34 -0.00
35 -0.0247   36 -0.0090   37 -0.0165   38  0.0203   39  0.0007   40  0.0216   41  0.0087
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ROW  26
26   1.0000   27  0.0197   28  0.0128   29 -0.0090   30  0.0065   31  0.0047   32 -0.0165   33  0.0413   34  0.0015   35 -0.0189
36  -0.0188   37 -0.0269   38  0.0011   39  0.0283   40 -0.0302   41 -0.0060

ROW  27
27   1.0000   28 -0.0238   29  0.0517   30 -0.0244   31  0.0182   32 -0.0197   33 -0.0038   34 -0.0111   35  0.0165   36 -0.0113
37   0.0201   38 -0.0158   39  0.0015   40  0.0408   41  0.0087

ROW  28
28   1.0000   29  0.0165   30  0.0014   31 -0.0002   32 -0.0275   33 -0.0025   34 -0.0087   35 -0.0289   36  0.0146   37 -0.0177
38   0.0042   39  0.0016   40  0.0034   41  0.0374

ROW  29
29   1.0000   30 -0.1752   31 -0.2725   32 -0.0149   33  0.0108   34 -0.0133   35  0.0231   36  0.0000   37  0.0326   38  0.0073
39  -0.0345   40 -0.0100   41 -0.0025

ROW  30
30   1.0000   31 -0.2496   32 -0.0253   33 -0.0186   34  0.0040   35 -0.0182   36  0.0282   37 -0.1435   38  0.0055   39 -0.0151
40  -0.0032   41  0.0156

ROW  31
31   1.0000   32  0.0090   33  0.0206   34  0.0184   35 -0.0387   36  0.0111   37 -0.0007   38  0.0151   39  0.0086   40  0.0341
41  -0.0219

ROW  32
32   1.0000   33  0.0215   34 -0.0100   35  0.0010   36 -0.0143   37 -0.0097   38  0.0147   39 -0.0322   40  0.0174   41  0.0254

ROW  33
33   1.0000   34 -0.0146   35  0.0038   36 -0.0407   37 -0.0083   38 -0.0123   39  0.0013   40  0.0208   41 -0.0027

ROW  34
34   1.0000   35  0.0099   36  0.0055   37 -0.0341   38  0.0044   39 -0.0356   40 -0.0040   41 -0.0417

ROW  35
35   1.0000   36 -0.0095   37  0.0194   38  0.0196   39 -0.0035   40  0.0645   41 -0.0029

ROW  36
36   1.0000   37 -0.1712   38 -0.2613   39  0.0258   40  0.0005   41 -0.0011

ROW  37
37   1.0000   38 -0.2559   39  0.0079   40 -0.0073   41  0.0389

ROW  38
38   1.0000   39 -0.0035   40  0.0061   41  0.0119

ROW  39
39   1.0000   40  0.0228   41  0.0133

ROW  40
40   1.0000   41  0.0019

ROW  41
41   1.0000
```

RFINE F051TE49 FINAL CYCLE

CORRELATION COEFICIENTS WITH LARGEST MAGNITUDES

PARAMETERS		VALUE	PARAMETERS		VALUE	PARAMETERS		VALUE	PARAMETERS		VALUE
2	5	-0.5502	2	3	-0.5401	2	4	-0.5066	1	2	-0.3154
23	25	-0.2834	29	31	-0.2725	17	19	-0.2666	11	13	-0.2630
36	38	-0.2613	37	38	-0.2559	18	24	-0.2530	12	13	-0.2521
18	19	-0.2510	30	31	-0.2496	24	25	-0.2405	17	18	-0.2000
23	24	-0.1947	16	22	-0.1912	19	25	-0.1760	29	30	-0.1752

RFINE FO51TE49 FINAL CYCLE
BOND DISTANCES BETWEEN, 1.50 AND 2.50 ANG.

ATOM 1	X	Y	Z	ATOM 2	X	Y	Z	DISTANCE	NUMBER
M1	0.0	0.0	0.0	O1	-0.24150	0.08671	0.25000	2.12392	1
				O1	0.24150	-0.08671	-0.25000	2.12392	2
				O2	-0.26995	0.05111	-0.25000	2.07496	3
				O2	0.26995	-0.05111	0.25000	2.07496	4
				O3	0.27818	0.15896	0.03742	2.14757	5
				O3	-0.27818	-0.15896	-0.03742	2.14757	6
									7
M2	0.98704	0.27904	0.25000	O1	0.75850	0.08671	0.25000	2.29598	8
				O2	1.23005	0.44889	0.25000	2.12898	9
				O3	1.27818	0.15896	0.03742	2.28674	10
				O3	0.77818	0.34104	-0.03742	2.12671	11
				O3	0.77818	0.34104	0.53742	2.12671	12
				O3	1.27818	0.15896	0.46258	2.28674	13
									14
SI	0.42262	0.09099	0.25000	O2	0.26995	-0.05111	0.25000	1.66074	15
				O3	0.27818	0.15896	0.03742	1.63771	5
				O1	0.75850	0.08671	0.25000	1.61083	6
				O3	0.27818	0.15896	0.46258	1.63771	9
									16
O1	0.75850	0.08671	0.25000	M2	0.98704	0.27904	0.25000	2.29598	9
				SI	0.42262	0.09099	0.25000	1.61083	8
				M1	1.00000	0.0	0.0	2.12392	15
				M1	1.00000	0.0	0.50000	2.12392	17
									18
O2	0.23005	0.44889	0.25000	M1	0.50000	0.50000	0.0	2.07496	19
				M1	0.50000	0.50000	0.50000	2.07496	20
				M2	-0.01296	0.27904	0.25000	2.12898	21
				SI	0.07738	0.59099	0.25000	1.66074	22
									23
O3	0.27818	0.15896	0.03742	M1	0.0	0.0	0.0	2.14757	6
				SI	0.42262	0.09099	0.25000	1.63771	1
				M2	-0.01296	0.27904	0.25000	2.28675	15
				M2	0.48704	0.22096	-0.25000	2.12670	22
									24

RFINE F051TE49 FINAL CYCLE

BOND ANGLES

CENTRAL ATOM	X	Y	Z
M1	0.0	0.0	0.0

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
O1	2	O1	3	179.980
O1	2	O2	4	94.649
O1	2	O2	5	85.351
O1	2	O3	6	85.929
O1	2	O3	7	94.071
O1	3	O2	4	85.351
O1	3	O2	5	94.649
O1	3	O3	6	94.071
O1	3	O3	7	85.929
O2	4	O2	5	180.000
O2	4	O3	6	105.389
O2	4	O3	7	74.611
O2	5	O3	6	74.611
O2	5	O3	7	105.389
O3	6	O3	7	179.956

CENTRAL ATOM	X	Y	Z
M2	0.98704	0.27904	0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
O1	9	O2	10	175.326
O1	9	O3	11	78.880
O1	9	O3	12	92.529
O1	9	O3	13	92.529
O1	9	O3	14	78.880
O2	10	O3	11	97.302
O2	10	O3	12	90.093
O2	10	O3	13	90.093
O2	10	O3	14	97.302
O3	11	O3	12	89.131
O3	11	O3	13	157.953
O3	11	O3	14	69.388
O3	12	O3	13	111.690
O3	12	O3	14	157.953
O3	13	O3	14	89.131

CENTRAL ATOM	X	Y	Z
SI	0.42262	0.09099	0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
O2	5	O3	6	101.800
O2	5	O1	9	114.552
O2	5	O3	16	101.800
O3	6	O1	9	115.772
O3	6	O3	16	105.267
O1	9	O3	16	115.772

CENTRAL ATOM

CENTRAL ATOM	X	Y	Z
01	0.75850	0.08671	0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M2	8	SI	15	116.904
M2	8	M1	17	96.677
M2	8	M1	18	96.677
SI	15	M1	17	123.836
SI	15	M1	18	123.836
M1	17	M1	18	92.228

CENTRAL ATOM	X	Y	Z
02	0.23005	0.44889	0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M1	20	M1	21	95.076
M1	20	M2	22	123.888
M1	20	SI	23	92.460
M1	21	M2	22	123.888
M1	21	SI	23	92.460
M2	22	SI	23	120.674

CENTRAL ATOM	X	Y	Z
03	0.27818	0.15896	0.03742

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M1	1	SI	15	90.531
M1	1	M2	22	96.286
M1	1	M2	24	116.204
SI	15	M2	22	92.611
SI	15	M2	24	126.285
M2	22	M2	24	126.149

RFINE F051TE49 FINAL CYCLE

ELLIPSOIDS OF VIBRATION

ELLIPSOID FOR M1

EQUIVALENT ISOTROPIC B = 0.4155

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.056096	31.14	60.89	60.50
2	0.068756	58.87	106.86	143.65
3	0.088962	90.88	160.70	70.75

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM M1 AT 0.0 0.0 0.0

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
O1	-0.24150	0.08671	0.25000	2.12392	2.12393	2.12431	2.12948	2.13503	0.06931
O1	0.24150	-0.08671	-0.25000	2.12392	2.12393	2.12431	2.12948	2.13503	0.06931
O2	-0.26995	0.05111	-0.25000	2.07496	2.07496	2.07516	2.08070	2.08643	0.06555
O2	0.26995	-0.05111	0.25000	2.07496	2.07496	2.07516	2.08070	2.08643	0.06555
O3	0.27818	0.15896	0.03742	2.14757	2.14759	2.14807	2.15285	2.15811	0.07437
O3	-0.27818	-0.15896	-0.03742	2.14757	2.14759	2.14807	2.15285	2.15811	0.07437

ELLIPSOID FOR M2

EQUIVALENT ISOTROPIC B = 0.5412

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.078267	58.70	148.70	90.00
2	0.083378	90.00	90.00	180.00
3	0.086522	31.29	58.71	90.00

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM M2 AT 0.98704 0.27904 0.25000

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
O1	0.75850	0.08671	0.25000	2.29598	2.29600	2.29642	2.30139	2.30678	0.08451
O2	1.23005	0.44889	0.25000	2.12898	2.12898	2.12900	2.13527	2.14155	0.08505
O3	1.27818	0.15896	0.03742	2.28674	2.28676	2.28722	2.29243	2.29809	0.08043
O3	0.77818	0.34104	-0.03742	2.12671	2.12671	2.12688	2.13302	2.13933	0.08229
O3	0.77818	0.34104	0.53742	2.12671	2.12671	2.12688	2.13302	2.13933	0.08229
O3	1.27818	0.15896	0.46258	2.28674	2.28676	2.28722	2.29243	2.29809	0.08043

ELLIPSOID FOR SI

EQUIVALENT ISOTROPIC B = 0.3625

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.060183	3.23	93.23	90.00
2	0.069116	90.00	90.00	180.00
3	0.073309	86.77	3.23	90.00

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM SI AT 0.42262 0.09099 0.25000

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
O2	0.26995	-0.05111	0.25000	1.66074	1.66079	1.66150	1.66671	1.67264	0.07147
O3	0.27818	0.15896	0.03742	1.63771	1.63783	1.63895	1.64452	1.65122	0.06817
O1	0.75850	0.08671	0.25000	1.61083	1.61106	1.61275	1.61906	1.62705	0.06019
O3	0.27818	0.15896	0.46258	1.63771	1.63783	1.63895	1.64452	1.65122	0.06817

ELLIPSOID FOR O1

EQUIVALENT ISOTROPIC B = 0.4984

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.050403	3.35	86.65	90.00
2	0.083315	90.00	90.00	180.00
3	0.097243	93.35	3.35	90.00

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O1 AT 0.75850 0.08671 0.25000

ATOM	X	Y	Z	DISTANCES RAW	LOWER	RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
M2	0.98704	0.27904	0.25000	2.29598	2.29600	2.29642	2.30139	2.30678	0.08677
SI	0.42262	0.09099	0.25000	1.61083	1.61106	1.61275	1.61906	1.62705	0.05091
M1	1.00000	0.0	0.0	2.12392	2.12393	2.12431	2.12948	2.13503	0.07929
M1	1.00000	0.0	0.50000	2.12392	2.12393	2.12431	2.12948	2.13503	0.07929

ELLIPSOID FOR O2

EQUIVALENT ISOTROPIC B = 0.4756

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.063236	28.96	61.04	90.00
2	0.083078	118.96	28.96	90.00
3	0.084681	90.00	90.00	0.0

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O2 AT 0.25005 0.44869 0.25000

ATOM	X	Y	Z	DISTANCES RAW	LOWER	RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
M1	0.50000	0.50000	0.0	2.07496	2.07496	2.07516	2.08070	2.08643	0.07578
M1	0.50000	0.50000	0.50000	2.07496	2.07496	2.07516	2.08070	2.08643	0.07578
M2	-0.01296	0.27904	0.25000	2.12898	2.12898	2.12900	2.13527	2.14155	0.06807
SI	0.07738	0.59099	0.25000	1.66074	1.66079	1.66150	1.66671	1.67264	0.08304

ELLIPSOID FOR O3

EQUIVALENT ISOTROPIC B = 0.4978

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.067708	1.34	89.69	88.69
2	0.077061	89.17	51.75	141.73
3	0.091604	91.05	38.26	51.76

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O3 AT 0.27818 0.15896 0.03742

ATOM	X	Y	Z	DISTANCES RAW	LOWER	RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
M1	0.0	0.0	0.0	2.14757	2.14759	2.14807	2.15285	2.15811	0.08055
SI	0.42262	0.09099	0.25000	1.63771	1.63783	1.63895	1.64452	1.65122	0.07568
M2	-0.01296	0.27904	0.25000	2.28675	2.28677	2.28723	2.29243	2.29809	0.08375
M2	0.48704	0.22096	-0.25000	2.12670	2.12671	2.12687	2.13302	2.13933	0.07651

PARAMETERS WRITTEN OUT TO UNIT 10.

SUMMARY OF ERRORS FOR THIS JOB	ERROR NUMBER	NUMBER OF ERRORS
	209	1

```
HASP JOB NO. = 8207   SYSTEM ENTRY          TIME = 10.47.02   DATE = AUG 15, 1979
                             PURGE                 10.49.33          AUG 15, 1979
   B0020CAF  310D3

JOB ACCOUNTING SUMMARY     START TIME ON MAIN   10.47.47

   EXECUTION TIME ON CPU1                        00.00.11
   DISK EXCPS                                        255           .61
   TAPE EXCPS                                          0           .05
   KILOBYTE SECONDS                                11552           .00
                                                                   .22
   CARD INPUT ON READER2                              51
                                                                   .08
   CARDS PUNCHED

   LINES PRINTED
      LOCAL
                                                    1460          1.02
   PLOTTER CHARGES

   PRIORITY CHARGES

                                          STANDARD EXECUTION       .00
                                          STANDARD OUTPUT          .00
   SETUPS

   TOTAL RUN CHARGES
                                                                  1.99
CURRENT BALANCE
                                                              1,166.50
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RFINE 108206  CYCLE  4
 CONTROL PARAMETERS ARE
1 1 1 2 2 0 0 0 0 0 0 0 0 0 0   0.0   0.0  0 0 0  0  0  0 0 0 0 0   0.0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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TE 91 FINAL CYCLE

RFINE 108206 CYCLE 4 STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
0	2	0	26.742	24.929	25.677	-0.144	1.812	30.9051	0.9426	
0	4	0	54.775	58.405	63.093	4.176	-3.630	-42.2599	0.8532	
0	6	0	13.351	13.403	13.412	0.872	-0.053	-0.4289	0.9946	
0	8	0	31.125	31.480	31.748	2.257	-0.355	-2.9262	0.9782	
0	10	0	54.580	53.983	55.2[illegible]	2.969	0.597	4.5010	0.9504	
0	12	0	27.593	27.592	27.743	0.428	0.001	0.0075	0.9889	
0	14	0	31.887	31.913	31.945	3.424	-0.026	-0.1444	0.9867	
0	16	0	29.542	26.793	-26.901	-0.855	2.750	13.9472	0.9910	
0	2	1	30.254	30.614	-31.668	0.785	-0.360	-6.8007	0.9340	
0	3	1	1.121 *	0.000	0.000	-0.000	1.121	1.9999	1.0000	* **
0	4	1	55.688	58.804	-63.315	-2.097	-3.116	-49.3502	0.8617	
0	6	1	80.648	82.250	90.738	2.651	-1.602	-21.8544	0.8210	
0	8	1	11.149	9.326	-9.041	-2.327	1.822	17.1449	0.9981	
0	10	1	51.967	52.084	53.264	2.501	-0.117	-1.2299	0.9541	
0	12	1	44.086	43.151	-43.699	-1.970	0.935	8.7215	0.9731	
0	14	1	12.444	11.166	-11.143	0.841	1.278	8.7107	0.9984	
0	16	1	4.385	4.512	-4.509	-0.181	-0.127	-0.3856	0.9997	
0	0	2	47.917	50.873	-54.689	-0.728	-2.957	-49.9570	0.8652	
0	2	2	63.726	71.704	80.468	4.844	-7.979	-133.8489	0.7912	
0	3	2	1.168 *	0.000	-0.000	-0.000	1.168	2.4514	1.0000	* **
0	4	2	21.300	22.934	23.135	0.479	-1.634	-23.1703	0.9823	
0	6	2	115.515	118.908	141.453	3.653	-3.393	-45.4932	0.7062	
0	8	2	37.289	38.965	39.497	1.929	-1.676	-19.6131	0.9709	
0	10	2	8.710	8.554	-8.512	0.891	0.156	1.2151	0.9988	
0	12	2	44.291	44.793	45.256	3.147	-0.502	-4.7524	0.9732	
0	14	2	6.641	6.276	6.273	-0.235	0.365	1.8327	0.9995	
0	16	2	47.829	45.035	45.447	3.543	2.793	21.5873	0.9760	
0	2	3	8.264	8.244	-8.217	-0.766	0.019	0.2342	0.9979	
0	3	3	1.258 *	0.000	0.000	0.000	1.258	1.9996	1.0000	* **
0	4	3	66.398	71.691	76.418	2.099	-5.293	-75.2408	0.8794	
0	6	3	62.273	66.604	-69.610	-2.470	-4.331	-56.0484	0.9144	
0	8	3	6.684	6.946	-6.561	2.289	-0.262	-1.9339	0.9992	
0	10	3	33.951	35.448	-35.687	-2.274	-1.497	-15.5834	0.9827	
0	12	3	42.481	43.320	43.773	2.015	-0.839	-7.9665	0.9773	
0	14	3	4.138	3.158	3.075	-0.719	0.981	3.7602	0.9999	
0	16	3	10.586	9.945	9.946	0.308	0.641	4.0162	0.9989	
0	0	4	136.168	143.828	181.981	5.262	-7.660	-105.1205	0.6241	
0	2	4	19.489	19.748	19.832	-0.115	-0.259	-3.4225	0.9915	
0	3	4	0.715 *	0.000	-0.000	0.000	0.714	0.7036	1.0000	* **
0	4	4	47.203	50.354	51.456	3.872	-3.151	-41.5156	0.9523	
0	6	4	2.411	2.465	-2.334	0.793	-0.054	-0.1929	0.9999	
0	8	4	26.255	27.515	27.583	2.099	-1.260	-13.3518	0.9894	
0	10	4	45.800	47.403	47.985	2.762	-1.603	-16.5342	0.9727	
0	12	4	17.457	17.870	17.897	0.391	-0.413	-3.5751	0.9964	
0	14	4	28.265	28.483	28.430	3.173	-0.218	-1.8255	0.9914	
0	2	5	25.219	26.694	-26.848	0.691	-1.475	-18.3293	0.9879	
0	3	5	1.773 *	0.000	-0.000	-0.000	1.773	3.8612	1.0000	* **
0	4	5	26.943	28.072	-28.183	-1.792	-1.129	-13.6501	0.9881	
0	6	5	52.464	56.060	57.219	2.422	-3.596	-42.0623	0.9582	
0	8	5	12.434	13.823	-13.693	-2.004	-1.388	-12.9812	0.9977	
0	10	5	42.634	44.171	44.588	2.332	-1.537	-15.3545	0.9787	
0	12	5	29.258	29.200	-29.283	-1.637	0.059	0.5331	0.9912	
0	14	5	12.739	12.360	-12.341	0.833	0.379	2.6382	0.9985	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
0	0	6	40.185		39.495	-39.913	-0.641	0.690	7.8526	0.9789	
0	2	6	48.868		50.602	51.328	4.156	-1.734	-20.4083	0.9656	
0	3	6	1.099	*	0.000	-0.000	-0.000	1.099	1.4490	1.0000	* **
0	4	6	21.777		22.376	22.441	0.443	-0.599	-6.6028	0.9938	
0	6	6	62.115		65.264	66.808	3.099	-3.149	-34.7927	0.9523	
0	8	6	26.443		27.038	27.092	1.669	-0.595	-6.0089	0.9922	
0	10	6	1.325	*	0.829	0.250	0.791	0.495	0.7755	1.0000	* **
0	12	6	26.109		26.035	25.983	2.672	0.074	0.6228	0.9934	
0	2	7	3.894		3.451	-3.397	-0.612	0.442	2.4791	0.9999	
0	3	7	1.474	*	0.000	0.000	0.000	1.474	2.5652	1.0000	* **
0	4	7	40.174		40.788	41.109	1.771	-0.614	-6.5869	0.9826	
0	6	7	34.253		34.875	-35.035	-1.961	-0.622	-6.3575	0.9878	
0	8	7	5.281		4.864	-4.463	1.935	0.417	2.3454	0.9998	
0	10	7	19.733		19.427	-19.381	-1.769	0.306	2.6830	0.9965	
0	12	7	31.453		30.420	30.501	1.749	1.033	8.8679	0.9914	
0	0	8	72.651		68.930	70.417	4.126	3.721	38.1884	0.9549	
0	2	8	14.273		13.321	13.332	-0.055	0.953	8.7950	0.9983	
0	3	8	0.785	*	0.000	-0.000	-0.000	0.785	0.6613	1.0000	* **
0	4	8	31.461		31.129	31.119	3.080	0.332	3.3311	0.9909	
0	6	8	9.993		9.789	-9.774	0.609	0.204	1.5796	0.9991	
0	8	8	19.662		18.570	18.522	1.682	1.092	9.3156	0.9969	
0	10	8	34.727		32.956	33.042	2.217	1.771	15.7118	0.9903	
0	2	9	10.914		9.984	-9.974	0.541	0.929	7.1167	0.9991	
0	4	9	16.572		14.953	-14.909	-1.326	1.619	14.2754	0.9980	
0	6	9	31.624		29.691	29.746	1.882	1.933	17.7518	0.9924	
0	0	10	28.278		24.298	-24.354	-0.473	3.980	23.3691	0.9950	
0	2	10	32.212		28.784	28.727	3.048	3.429	30.4399	0.9928	
1	1	0	19.186		17.998	18.190	1.663	1.189	15.1025	0.9708	
1	2	0	28.760		26.965	-27.726	-0.203	1.794	19.8445	0.9458	
1	3	0	112.791		97.605	128.669	3.964	15.186	162.4200	0.5749	
1	4	0	61.065		55.620	59.739	0.139	5.445	56.2971	0.8669	
1	5	0	31.445		30.911	31.458	0.286	0.534	5.1233	0.9654	
1	6	0	16.551		16.548	16.617	-0.117	0.003	0.0268	0.9917	
1	7	0	101.040		98.391	111.122	4.895	2.649	23.0942	0.7825	
1	8	0	7.314		7.449	-7.448	0.274	-0.134	-0.6887	0.9988	
1	9	0	13.475		13.391	-13.400	-0.633	0.084	0.5412	0.9965	
1	10	0	8.116		8.566	8.570	-0.131	-0.450	-2.1432	0.9987	
1	11	0	43.497		43.507	44.001	3.780	-0.010	-0.0721	0.9705	
1	12	0	1.665	*	0.118	-0.089	0.078	1.547	1.8578	1.0000	* **
1	13	0	5.150		2.825	2.816	0.236	2.325	7.2327	0.9999	
1	14	0	16.819		16.277	-16.304	-0.201	0.543	2.8155	0.9965	
1	15	0	38.926		37.221	37.483	2.284	1.706	9.3963	0.9824	
1	16	0	1.910	*	2.012	2.012	0.042	-0.102	-0.1064	0.9999	* **
1	0	1	25.144		25.149	-25.712	0.089	-0.005	-0.0811	0.9566	
1	1	1	56.587		54.130	-60.129	-2.652	2.457	40.6530	0.8088	
1	2	1	17.935		16.777	-16.936	-0.252	1.157	16.2440	0.9812	
1	3	1	87.840		79.033	93.439	2.621	8.807	128.8349	0.7149	
1	4	1	0.787	*	1.167	1.143	0.235	-0.380	-0.5495	0.9999	* **
1	5	1	38.409		37.491	-38.389	-1.564	0.919	12.3050	0.9522	
1	6	1	7.771		7.008	-7.013	-0.008	0.763	6.5744	0.9986	
1	7	1	10.341		9.540	-9.540	0.462	0.801	7.4004	0.9977	
1	8	1	7.613		7.856	7.862	0.028	-0.243	-1.7964	0.9987	
1	9	1	11.172		11.101	-11.113	0.189	0.071	0.6022	0.9976	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	10	1	8.661	8.465	8.470	-0.003	0.196	1.4006	0.9988	
1	11	1	12.427	12.141	-12.105	-1.098	0.286	2.2632	0.9977	
1	12	1	1.797 *	0.924	0.912	-0.152	0.872	1.5785	1.0000	* **
1	13	1	39.411	37.695	38.011	1.991	1.716	14.6937	0.9807	
1	14	1	7.585	7.162	7.162	0.202	0.423	2.1898	0.9993	
1	15	1	17.527	16.407	-16.327	-1.886	1.120	7.8540	0.9965	
1	16	1	2.280 *	1.192	1.189	-0.073	1.089	1.9000	1.0000	* **
1	1	2	92.035	91.313	110.172	3.107	0.722	11.0333	0.6864	
1	2	2	48.148	43.045	-45.012	0.125	5.103	72.0772	0.9145	
1	3	2	30.451	28.299	28.756	0.798	2.152	29.1998	0.9677	
1	4	2	1.806	2.034	2.033	-0.068	-0.228	-0.7178	0.9999	
1	5	2	69.185	68.586	73.315	4.219	0.598	7.8702	0.8723	
1	6	2	6.676	6.945	-6.948	0.129	-0.270	-2.1326	0.9988	
1	7	2	19.458	20.265	-20.352	-0.532	-0.807	-8.8466	0.9908	
1	8	2	26.228	27.769	-27.975	-0.339	-1.540	-16.7967	0.9852	
1	9	2	84.470	84.601	89.887	4.629	-0.131	-1.4186	0.8835	
1	10	2	10.638	11.217	11.227	0.180	-0.580	-4.5377	0.9980	
1	11	2	12.293	12.654	12.669	-0.048	-0.361	-2.8718	0.9976	
1	12	2	6.562	6.805	6.807	-0.053	-0.244	-1.3861	0.9994	
1	13	2	38.006	37.711	37.938	3.058	0.295	2.5510	0.9817	
1	14	2	1.479 *	1.420	-1.413	0.141	0.059	0.0801	1.0000	* **
1	15	2	3.086	2.347	2.241	0.696	0.739	1.8741	0.9999	
1	16	2	6.613	6.361	6.362	-0.008	0.252	1.1343	0.9995	
1	0	3	14.245	13.627	-13.664	-0.112	0.618	8.4005	0.9946	
1	1	3	50.041	50.965	52.968	2.568	-0.924	-13.0100	0.9236	
1	2	3	27.524	26.650	26.967	0.275	0.874	11.3411	0.9765	
1	3	3	69.568	68.938	-74.018	-2.481	0.630	8.3874	0.8665	
1	4	3	12.641	12.237	12.260	-0.190	0.404	4.5469	0.9960	
1	5	3	26.082	27.208	27.403	1.554	-1.126	-13.8018	0.9826	
1	6	3	14.829	15.822	-15.862	-0.019	-0.994	-10.7470	0.9950	
1	7	3	13.178	13.533	13.551	-0.356	-0.355	-3.5273	0.9967	
1	8	3	1.403 *	0.947	-0.947	-0.003	0.456	0.8565	1.0000	* **
1	9	3	11.722	12.211	12.225	-0.083	-0.489	-4.3331	0.9977	
1	10	3	1.221 *	1.722	1.722	0.038	-0.501	-0.7663	1.0000	* **
1	11	3	11.544	10.019	9.958	1.155	1.525	12.2762	0.9987	
1	12	3	9.941	10.207	-10.213	0.126	-0.266	-1.8487	0.9987	
1	13	3	31.381	31.524	-31.656	-1.794	-0.143	-1.2302	0.9885	
1	14	3	4.676	4.844	-4.841	-0.180	-0.168	-0.6586	0.9997	
1	15	3	17.752	17.258	17.179	1.932	0.493	3.6210	0.9967	
1	16	3	4.614	4.356	4.355	0.098	0.258	0.9264	0.9998	
1	1	4	14.280	14.351	14.301	1.544	-0.071	-0.8301	0.9955	
1	2	4	6.216	6.980	-6.982	-0.171	-0.764	-6.1047	0.9988	
1	3	4	74.259	76.023	80.879	3.663	-1.764	-22.2079	0.8817	
1	4	4	20.226	21.792	21.899	0.111	-1.565	-18.2715	0.9902	
1	5	4	24.416	25.118	25.266	0.276	-0.702	-8.1642	0.9882	
1	6	4	8.412	9.676	9.683	-0.109	-1.264	-10.6746	0.9984	
1	7	4	76.756	79.575	83.341	4.530	-2.819	-32.2262	0.9090	
1	8	4	2.406	2.812	2.799	0.271	-0.405	-1.2817	0.9999	
1	9	4	11.686	12.297	-12.296	-0.580	-0.611	-5.3534	0.9980	
1	10	4	2.446	2.508	2.505	-0.132	-0.063	-0.1892	0.9999	
1	11	4	34.910	35.873	35.973	3.498	-0.963	-9.1587	0.9851	
1	12	4	0.498 *	1.147	-1.145	0.068	-0.650	-0.3547	1.0000	* **
1	13	4	4.091	3.085	3.076	0.229	1.007	3.9981	0.9999	

RFINE 108206 CYCLE 4

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	14	4	9.996	10.091	-10.095	-0.172	-0.095	-0.6164	0.9989	
1	15	4	31.291	31.202	31.293	2.116	0.088	0.7031	0.9897	
1	0	5	24.861	26.245	-26.391	0.061	-1.383	-17.0161	0.9889	
1	1	5	28.288	28.166	-28.281	-2.332	0.122	1.4310	0.9852	
1	2	5	2.728	2.622	-2.614	-0.198	0.106	0.4248	0.9999	
1	3	5	53.632	55.019	56.363	2.362	-1.387	-16.4309	0.9512	
1	4	5	10.260	11.081	11.089	0.239	-0.820	-7.8856	0.9981	
1	5	5	23.729	23.503	-23.559	-1.336	0.226	2.5319	0.9921	
1	6	5	11.424	11.742	-11.753	-0.020	-0.318	-3.0528	0.9981	
1	7	5	4.610	4.440	-4.414	0.487	0.170	0.9846	0.9997	
1	8	5	7.455	7.688	7.691	0.044	-0.233	-1.7322	0.9993	
1	9	5	6.400	6.374	-6.371	0.257	0.025	0.1646	0.9995	
1	10	5	10.476	10.804	10.811	0.023	-0.328	-2.5555	0.9987	
1	11	5	9.023	9.292	-9.255	-0.877	-0.270	-1.8951	0.9991	
1	12	5	4.912	5.319	-5.317	-0.148	-0.406	-1.8485	0.9997	
1	13	5	31.605	31.126	31.223	1.878	0.478	4.0899	0.9902	
1	14	5	6.975	6.548	6.546	0.192	0.427	2.3426	0.9996	
1	1	6	56.946	56.870	58.107	2.668	0.076	0.8688	0.9559	
1	2	6	3.018	1.823	-1.818	0.137	1.195	5.4001	1.0000	
1	3	6	10.523	10.487	10.472	0.687	0.036	0.3391	0.9986	
1	4	6	6.620	6.541	-6.542	-0.080	0.079	0.5872	0.9995	
1	5	6	38.560	39.557	39.786	3.608	-0.997	-10.7863	0.9805	
1	6	6	4.029	5.087	-5.087	0.106	-1.058	-5.4060	0.9997	
1	7	6	10.348	10.949	-10.948	-0.435	-0.601	-3.6804	0.9987	
1	8	6	8.294	8.776	-8.775	-0.264	-0.482	-3.6270	0.9992	
1	9	6	54.199	55.253	56.004	3.956	-1.054	-10.3368	0.9686	
1	10	6	3.561	1.551	1.545	0.134	2.010	7.9985	1.0000	
1	11	6	8.981	8.803	8.806	-0.019	0.178	1.2301	0.9992	
1	12	6	3.056	3.009	3.009	-0.049	0.047	0.1500	0.9999	
1	13	6	29.001	28.751	28.747	2.627	0.250	2.0869	0.9920	
1	0	7	6.627	6.109	-6.109	-0.088	0.519	4.1509	0.9996	
1	1	7	24.671	24.144	24.134	2.112	0.526	5.4912	0.9932	
1	2	7	13.218	13.330	13.341	0.242	-0.112	-1.0750	0.9980	
1	3	7	37.816	37.608	-37.846	-2.003	0.208	2.1712	0.9847	
1	4	7	5.595	5.496	5.495	-0.140	0.099	0.6394	0.9997	
1	5	7	14.360	14.214	14.168	1.320	0.146	1.3538	0.9979	
1	6	7	11.296	11.734	-11.742	-0.017	-0.438	-3.7617	0.9986	
1	7	7	9.485	9.057	9.058	-0.220	0.428	3.3472	0.9992	
1	8	7	1.280 *	0.346	0.346	0.010	0.934	1.4597	1.0000	* **
1	9	7	8.408	8.278	8.281	0.016	0.130	0.8948	0.9994	
1	10	7	3.209	3.199	3.199	0.051	0.010	0.0360	0.9999	
1	11	7	7.507	7.337	7.266	1.033	0.170	1.0376	0.9995	
1	12	7	9.366	8.921	-8.924	0.106	0.444	2.9525	0.9993	
1	1	8	7.770	7.501	7.401	1.233	0.270	1.9327	0.9995	
1	2	8	4.763	4.070	4.069	-0.109	0.693	3.8419	0.9998	
1	3	8	38.326	36.991	37.122	2.893	1.335	13.2016	0.9870	
1	4	8	1.219 *	1.247	1.246	0.059	-0.029	-0.0469	1.0000	* **
1	5	8	14.671	14.005	14.016	0.244	0.665	5.8304	0.9982	
1	6	8	3.686	3.633	3.632	-0.088	0.053	0.2161	0.9999	
1	7	8	47.782	46.459	46.779	3.589	1.323	12.4773	0.9806	
1	8	8	9.367	9.084	9.084	0.245	0.284	2.0660	0.9992	
1	9	8	9.077	8.476	-8.468	-0.444	0.600	4.2310	0.9993	
1	10	8	3.609	3.656	-3.654	-0.121	-0.047	-0.1686	0.9999	

RFINE 108206 CYCLE 4 STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	0	9	10.423	10.313	-10.318	0.058	0.110	0.8968	0.9991	
1	1	9	15.090	13.956	-13.858	-1.751	1.135	9.9141	0.9982	
1	2	9	2.114	2.084	-2.079	-0.143	0.030	0.0790	1.0000	
1	3	9	29.596	27.679	27.713	1.817	1.917	17.6410	0.9933	
1	4	9	5.270	5.054	5.051	0.191	0.216	1.1745	0.9998	
1	5	9	12.200	11.316	-11.281	-0.964	0.885	7.0416	0.9988	
1	6	9	4.710	4.531	-4.532	0.003	0.179	0.8829	0.9998	
1	7	9	2.200	1.311	-1.242	0.421	0.889	2.2531	1.0000	
2	0	0	69.584	74.058	83.521	5.248	-4.474	-47.2587	0.7831	
2	1	0	40.585	40.546	42.054	0.567	0.039	0.3989	0.9294	
2	2	0	3.805	0.384	0.351	-0.156	3.421	10.4679	1.0000	
2	3	0	14.999	14.885	14.951	-0.154	0.114	0.9431	0.9910	
2	4	0	103.799	95.684	111.512	4.191	8.115	73.5285	0.7352	
2	5	0	8.881	8.142	-8.146	0.258	0.739	4.5768	0.9980	
2	6	0	2.806	2.181	1.971	0.934	0.625	1.4684	0.9999	
2	7	0	18.659	17.992	-18.061	-0.279	0.667	4.6078	0.9921	
2	8	0	56.865	53.803	55.478	2.254	3.061	22.1524	0.9390	
2	9	0	15.783	15.704	-15.740	-0.196	0.080	0.4801	0.9953	
2	10	0	65.142	62.795	64.898	2.859	2.347	15.6355	0.9344	
2	11	0	2.386 *	1.702	1.689	0.211	0.684	1.1083	1.0000	* **
2	12	0	5.466	2.452	2.431	0.324	3.014	9.5154	0.9999	
2	13	0	14.689	13.940	13.959	-0.067	0.749	3.7077	0.9973	
2	14	0	43.842	41.454	41.794	3.390	2.388	12.9957	0.9773	
2	15	0	11.561	11.141	11.143	0.388	0.420	1.7059	0.9984	
2	16	0	2.183 *	3.137	-3.067	-0.662	-0.954	-1.0630	0.9999	* **
2	1	1	33.517	33.088	33.846	0.123	0.429	6.0930	0.9557	
2	2	1	22.542	20.825	20.993	0.890	1.717	22.1447	0.9822	
2	3	1	1.877	0.269	0.194	0.186	1.608	4.5977	1.0000	
2	4	1	62.503	59.003	-62.443	-1.972	3.500	43.7027	0.8920	
2	5	1	30.512	29.976	-30.368	-0.539	0.536	6.1898	0.9741	
2	6	1	40.838	38.920	39.633	2.451	1.918	21.4510	0.9607	
2	7	1	4.946	4.759	-4.751	0.290	0.187	0.9301	0.9994	
2	8	1	40.773	38.679	-39.225	-2.383	2.095	20.8505	0.9688	
2	9	1	1.396 *	0.655	0.597	-0.269	0.741	1.0621	1.0000	* **
2	10	1	32.298	30.916	31.079	2.340	1.382	12.5646	0.9839	
2	11	1	17.769	17.089	17.121	0.504	0.680	5.4501	0.9955	
2	12	1	25.704	25.311	-25.365	-1.797	0.393	3.1539	0.9908	
2	13	1	3.037	2.440	-2.431	-0.209	0.597	1.4420	0.9999	
2	14	1	16.891	15.002	14.995	0.949	1.889	13.1088	0.9970	
2	15	1	9.860	8.901	-8.905	-0.037	0.960	5.1888	0.9990	
2	16	1	3.794	2.590	2.585	-0.153	1.204	3.4005	0.9999	
2	0	2	17.434	18.977	-19.076	-0.546	-1.542	-20.6339	0.9888	
2	1	2	11.546	12.406	-12.426	-0.524	-0.861	-10.2946	0.9952	
2	2	2	118.352	114.431	140.500	4.822	3.920	52.2831	0.6626	
2	3	2	12.086	12.141	-12.168	0.155	-0.055	-0.5819	0.9955	
2	4	2	33.119	32.288	32.751	0.452	0.831	10.0374	0.9717	
2	5	2	12.151	12.288	-12.308	-0.283	-0.137	-1.3186	0.9962	
2	6	2	50.061	48.061	49.223	3.338	2.000	22.3937	0.9490	
2	7	2	29.602	29.168	29.434	0.304	0.434	4.5123	0.9819	
2	8	2	31.160	29.935	30.132	1.882	1.224	12.1166	0.9832	
2	9	2	17.613	17.655	17.701	0.204	-0.042	-0.3703	0.9947	
2	10	2	14.555	13.737	13.721	1.008	0.818	6.6197	0.9970	
2	11	2	11.326	11.177	-11.185	-0.231	0.149	1.0581	0.9982	

RFINE 108206 CYCLE 4

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
2	12	2	27.798	26.817	26.774	3.049	0.981	8.1638	0.9904	
2	13	2	8.418	7.859	-7.861	0.088	0.559	3.2002	0.9992	
2	14	2	3.512	0.532	-0.466	-0.256	2.981	8.5363	1.0000	
2	15	2	8.598	8.200	-8.195	-0.366	0.398	2.0531	0.9992	
2	16	2	43.962	42.915	43.246	3.375	1.047	7.7864	0.9788	
2	1	3	19.301	20.127	-20.227	-0.082	-0.825	-10.4367	0.9901	
2	2	3	7.274	6.350	6.303	-0.796	0.924	8.1717	0.9990	
2	3	3	9.805	9.724	-9.734	-0.170	0.080	0.7540	0.9978	
2	4	3	35.366	35.965	36.422	1.914	-0.599	-7.1158	0.9724	
2	5	3	29.568	30.214	30.493	0.551	-0.646	-7.3464	0.9815	
2	6	3	35.709	35.516	-35.859	-2.291	0.193	2.1094	0.9770	
2	7	3	9.029	9.208	9.212	-0.243	-0.179	-1.4074	0.9985	
2	8	3	46.688	46.626	47.386	2.407	0.062	0.6409	0.9657	
2	9	3	6.176	6.006	-6.002	0.266	0.170	1.0094	0.9995	
2	10	3	34.160	33.910	-34.107	-2.170	0.250	2.3195	0.9845	
2	11	3	13.934	13.797	-13.806	-0.460	0.137	1.0838	0.9975	
2	12	3	22.261	22.087	22.079	1.830	0.174	1.4279	0.9939	
2	13	3	5.018	5.260	5.256	0.230	-0.242	-0.9944	0.9997	
2	14	3	6.911	5.519	-5.466	-0.771	1.392	7.1547	0.9997	
2	15	3	5.288	5.282	5.282	0.042	0.006	0.0237	0.9997	
2	0	4	73.073	74.291	78.004	4.872	-1.218	-15.7642	0.9035	
2	1	4	22.229	23.130	23.239	0.517	-0.901	-10.9576	0.9901	
2	2	4	3.197	2.169	-2.164	-0.143	1.028	4.6049	0.9999	
2	3	4	11.588	12.124	12.139	-0.140	-0.536	-5.2438	0.9973	
2	4	4	65.871	67.454	70.074	3.866	-1.583	-18.3927	0.9238	
2	5	4	1.192 *	0.633	-0.582	0.247	0.559	0.9383	1.0000	* **
2	6	4	8.376	8.071	8.026	0.885	0.305	2.2737	0.9990	
2	7	4	16.577	16.810	-16.843	-0.265	-0.233	-2.2440	0.9958	
2	8	4	38.942	39.627	40.005	2.084	-0.685	-6.9142	0.9785	
2	9	4	12.894	12.923	-12.936	-0.183	-0.029	-0.2410	0.9978	
2	10	4	47.947	48.185	48.808	2.639	-0.238	-2.2317	0.9718	
2	11	4	3.655	3.419	3.413	0.203	0.236	0.8391	0.9999	
2	12	4	5.875	5.898	5.890	0.323	-0.023	-0.1124	0.9996	
2	13	4	10.562	10.181	10.187	-0.064	0.381	2.5328	0.9989	
2	14	4	35.582	35.183	35.272	3.135	0.399	3.1928	0.9871	
2	15	4	9.324	9.104	9.100	0.358	0.220	1.2693	0.9992	
2	1	5	22.438	22.907	22.998	0.143	-0.468	-5.3617	0.9921	
2	2	5	18.580	18.896	18.928	0.833	-0.315	-3.3516	0.9947	
2	3	5	4.734	5.112	-5.109	0.177	-0.377	-2.2957	0.9996	
2	4	5	44.598	45.424	-46.061	-1.726	-0.826	-9.1334	0.9712	
2	5	5	18.036	18.485	-18.521	-0.451	-0.449	-4.4662	0.9954	
2	6	5	26.999	27.184	27.221	2.236	-0.185	-1.8772	0.9906	
2	7	5	2.754	0.650	-0.584	0.286	2.104	7.3143	1.0000	
2	8	5	18.018	17.652	-17.571	-2.007	0.366	3.3539	0.9963	
2	9	5	3.175	2.417	-2.407	-0.226	0.757	2.6952	0.9999	
2	10	5	19.550	19.622	19.545	2.154	-0.072	-0.6256	0.9958	
2	11	5	13.669	13.586	13.591	0.472	0.083	0.6432	0.9980	
2	12	5	19.505	19.902	-19.886	-1.499	-0.397	-3.1914	0.9959	
2	13	5	1.422 *	0.189	0.100	-0.161	1.233	1.7340	1.0000	* **
2	14	5	18.327	18.175	18.179	0.965	0.152	1.1349	0.9968	
2	0	6	1.483 *	2.029	-1.984	-0.426	-0.547	-1.2705	1.0000	* **
2	1	6	13.500	13.501	-13.508	-0.460	-0.001	-0.0123	0.9978	
2	2	6	64.989	64.793	66.352	4.108	0.196	2.1158	0.9499	

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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	3	6	9.126	9.076	-9.080	0.129	0.050	0.4160	0.9990
2	4	6	13.626	13.102	13.110	0.386	0.524	4.8647	0.9980
2	5	6	2.705	2.942	-2.933	-0.229	-0.236	-0.8225	0.9999
2	6	6	41.016	40.653	40.943	2.889	0.363	3.6285	0.9810
2	7	6	15.004	14.869	14.885	0.253	0.135	1.1942	0.9977
2	8	6	17.348	16.851	16.799	1.610	0.496	4.3392	0.9971
2	9	6	11.028	10.859	10.864	0.176	0.169	1.2747	0.9988
2	10	6	5.842	5.029	4.956	0.857	0.813	4.4238	0.9997
2	11	6	5.083	4.765	-4.762	-0.185	0.319	1.5199	0.9998
2	12	6	26.135	25.363	25.307	2.634	0.772	6.3498	0.9937
2	13	6	7.266	6.936	-6.937	0.068	0.330	1.7945	0.9995
2	1	7	10.154	9.841	-9.846	-0.045	0.313	2.6903	0.9990
2	2	7	7.143	6.684	6.657	-0.618	0.459	3.2335	0.9995
2	3	7	5.113	5.131	-5.130	-0.120	-0.018	-0.1080	0.9997
2	4	7	19.103	18.866	18.832	1.602	0.237	2.2113	0.9964
2	5	7	18.275	17.758	17.779	0.478	0.517	4.7260	0.9969
2	6	7	21.146	20.891	-20.855	-1.821	0.255	2.3228	0.9958
2	7	7	6.403	6.276	6.275	-0.174	0.127	0.7654	0.9996
2	8	7	32.309	31.447	31.532	2.048	0.862	7.7922	0.9904
2	9	7	4.342	4.306	-4.300	0.231	0.036	0.1553	0.9998
2	10	7	22.910	22.581	-22.570	-1.698	0.330	2.7407	0.9953
2	11	7	8.388	8.142	-8.137	-0.361	0.246	1.5139	0.9994
2	0	8	52.194	49.495	49.904	3.884	2.699	27.2296	0.9778
2	1	8	8.651	7.988	7.980	0.397	0.663	5.1049	0.9994
2	2	8	4.432	4.270	-4.269	-0.105	0.162	0.7924	0.9998
2	3	8	6.882	6.226	6.226	-0.106	0.656	4.3488	0.9996
2	4	8	33.069	31.208	31.203	3.040	1.861	17.4264	0.9909
2	5	8	4.106	3.473	3.467	0.209	0.632	2.8780	0.9999
2	6	8	13.023	11.894	11.878	0.740	1.129	9.0717	0.9987
2	7	8	12.637	11.757	-11.763	-0.219	0.880	6.8289	0.9988
2	8	8	21.736	20.993	20.970	1.650	0.744	6.3066	0.9960
2	9	8	8.136	7.724	-7.725	-0.146	0.412	2.5472	0.9995
2	1	9	11.590	10.741	10.746	0.130	0.849	6.8628	0.9990
2	2	9	9.090	8.258	8.236	0.639	0.832	6.0222	0.9994
2	3	9	1.963	1.550	-1.542	0.155	0.414	1.0149	1.0000
2	4	9	23.506	22.057	-22.066	-1.267	1.450	12.7225	0.9958
2	5	9	10.290	9.262	-9.260	-0.328	1.028	7.4517	0.9992
2	6	9	17.029	15.453	15.370	1.741	1.576	13.1216	0.9980
3	1	0	54.051	52.870	55.011	1.796	1.181	10.4062	0.9227
3	2	0	32.114	32.324	-32.810	-0.473	-0.210	-1.7483	0.9704
3	3	0	69.517	65.686	69.748	3.674	3.831	31.1170	0.8845
3	4	0	44.544	44.049	-45.137	0.180	0.496	3.9440	0.9523
3	5	0	18.618	17.914	17.977	0.175	0.704	4.9448	0.9928
3	6	0	5.306	6.213	-6.199	-0.443	-0.906	-3.2101	0.9992
3	7	0	83.083	80.329	85.105	4.523	2.754	20.4320	0.8884
3	8	0	45.913	45.474	46.262	0.857	0.439	3.0822	0.9659
3	9	0	19.045	19.300	-19.350	-0.472	-0.255	-1.5841	0.9943
3	10	0	6.581	6.300	-6.285	-0.465	0.281	1.1420	0.9994
3	11	0	45.046	44.469	44.908	3.689	0.577	3.6065	0.9740
3	12	0	11.016	10.254	-10.259	0.230	0.761	3.5793	0.9987
3	13	0	6.464	6.501	6.496	0.293	-0.037	-0.1226	0.9995
3	14	0	8.496	7.262	-7.253	-0.394	1.234	4.9123	0.9994
3	15	0	19.964	19.527	19.466	2.009	0.437	2.1752	0.9957

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	0	1	13.766	14.028	-14.061	0.374	-0.263	-2.8157	0.9947
3	1	1	50.467	50.245	-51.945	-2.556	0.222	2.7397	0.9333
3	2	1	21.726	21.493	-21.619	-0.663	0.233	2.5781	0.9874
3	3	1	57.571	55.125	57.474	2.266	2.446	27.6410	0.9185
3	4	1	38.377	37.397	38.043	0.665	0.980	10.7639	0.9660
3	5	1	16.746	16.449	-16.435	-1.446	0.297	2.8902	0.9940
3	6	1	29.564	29.204	29.454	0.001	0.361	3.7053	0.9831
3	7	1	8.149	7.980	7.964	0.578	0.168	1.1670	0.9988
3	8	1	5.890	5.545	-5.547	0.026	0.345	1.8766	0.9995
3	9	1	3.453	2.852	2.835	0.311	0.601	2.1148	0.9999
3	10	1	27.588	27.372	-27.518	-0.090	0.216	1.8874	0.9894
3	11	1	11.831	11.640	-11.602	-1.056	0.191	1.3254	0.9982
3	12	1	19.897	19.393	-19.434	-0.466	0.504	3.8846	0.9953
3	13	1	19.817	19.552	19.525	1.691	0.264	1.9467	0.9954
3	14	1	9.716	9.166	9.156	0.512	0.550	3.1456	0.9990
3	15	1	22.032	21.365	-21.343	-1.819	0.667	4.7224	0.9948
3	1	2	60.965	62.342	65.138	2.799	-1.377	-17.1212	0.9143
3	2	2	59.450	60.228	62.847	0.522	-0.778	-9.3546	0.9183
3	3	2	1.847	1.442	1.198	0.802	0.405	0.9332	1.0000
3	4	2	14.539	14.945	14.978	-0.224	-0.406	-3.9267	0.9953
3	5	2	72.037	71.385	74.881	4.150	0.652	7.2075	0.9060
3	6	2	1.617 *	1.259	1.184	0.428	0.357	0.7122	1.0000 * **
3	7	2	3.971	3.146	3.131	-0.318	0.824	3.7070	0.9998
3	8	2	22.206	22.393	-22.465	-0.780	-0.187	-1.7514	0.9924
3	9	2	59.437	59.720	61.097	4.231	-0.284	-2.7271	0.9509
3	10	2	6.416	6.438	-6.426	0.425	-0.023	-0.1291	0.9995
3	11	2	8.370	7.998	8.000	-0.110	0.372	2.3628	0.9992
3	12	2	5.619	5.083	5.079	-0.233	0.535	2.4240	0.9997
3	13	2	40.051	40.345	40.618	2.891	-0.294	-2.4014	0.9816
3	14	2	19.405	19.095	19.128	0.439	0.310	2.2635	0.9960
3	15	2	5.431	4.512	4.442	0.790	0.920	3.8247	0.9998
3	0	3	28.687	29.766	30.014	-0.288	-1.079	-12.4212	0.9834
3	1	3	31.422	32.504	32.738	2.447	-1.082	-12.8301	0.9803
3	2	3	11.955	12.316	12.317	0.663	-0.362	-3.5050	0.9971
3	3	3	47.396	47.452	-48.431	-2.142	-0.055	-0.6130	0.9581
3	4	3	38.363	39.387	-39.918	-0.618	-1.024	-11.2471	0.9733
3	5	3	24.180	24.985	25.069	1.469	-0.804	-8.3770	0.9899
3	6	3	13.121	13.153	-13.171	0.065	-0.032	-0.2982	0.9974
3	7	3	11.684	12.412	-12.416	-0.496	-0.728	-6.1242	0.9978
3	8	3	2.250	2.132	2.132	0.001	0.118	0.3107	0.9999
3	9	3	3.552	2.621	-2.612	-0.211	0.931	3.5954	0.9999
3	10	3	19.038	19.255	19.297	0.101	-0.217	-1.8775	0.9956
3	11	3	17.602	17.785	17.780	1.137	-0.183	-1.5101	0.9965
3	12	3	24.466	24.613	24.689	0.500	-0.147	-1.2124	0.9935
3	13	3	20.134	20.216	-20.201	-1.527	-0.082	-0.6333	0.9957
3	14	3	9.491	9.176	-9.168	-0.470	0.316	1.9415	0.9991
3	1	4	33.809	34.594	34.878	1.659	-0.785	-9.0121	0.9816
3	2	4	29.578	30.523	-30.743	-0.450	-0.945	-10.4707	0.9855
3	3	4	56.068	55.564	56.826	3.411	0.504	5.5219	0.9527
3	4	4	25.660	26.505	-26.647	0.178	-0.846	-8.8793	0.9893
3	5	4	11.447	11.382	11.391	0.165	0.065	0.5761	0.9982
3	6	4	3.418	3.376	-3.352	-0.405	0.042	0.1799	0.9999
3	7	4	60.591	62.310	63.684	4.177	-1.719	-17.6023	0.9532

RFINE 108206 CYCLE 4

STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	8	4	31.376		31.993	32.175	0.781	-0.617	-6.0089	0.9881	
3	9	4	11.677		12.098	-12.101	-0.417	-0.422	-3.3372	0.9984	
3	10	4	2.367		2.448	-2.412	-0.418	-0.081	-0.2021	0.9999	
3	11	4	35.742		36.628	36.726	3.411	-0.886	-7.8247	0.9862	
3	12	4	7.564		7.470	-7.469	0.215	0.094	0.5381	0.9994	
3	13	4	4.191		3.978	3.969	0.274	0.213	0.8017	0.9998	
3	14	4	8.913		8.453	-8.448	-0.373	0.460	2.8252	0.9993	
3	0	5	2.746		1.847	-1.806	0.388	0.899	3.7243	1.0000	
3	1	5	37.029		37.815	-38.099	-2.270	-0.786	-8.6505	0.9817	
3	2	5	17.833		17.573	-17.599	-0.562	0.260	2.6403	0.9960	
3	3	5	36.832		36.423	36.701	2.041	0.409	4.2472	0.9819	
3	4	5	21.045		21.090	21.138	0.614	-0.045	-0.4460	0.9945	
3	5	5	5.986		5.677	-5.547	-1.213	0.308	1.9665	0.9996	
3	6	5	26.740		27.198	27.312	0.057	-0.457	-4.5225	0.9916	
3	7	5	3.037		2.573	2.509	0.571	0.464	1.6693	0.9999	
3	8	5	5.179		5.288	-5.288	0.049	-0.109	-0.5634	0.9997	
3	9	5	2.572		2.296	2.268	0.358	0.277	0.7781	0.9999	
3	10	5	22.834		23.360	-23.423	-0.064	-0.527	-4.5609	0.9946	
3	11	5	3.991		4.160	-4.077	-0.827	-0.169	-0.6325	0.9998	
3	12	5	10.277		10.106	-10.104	-0.370	0.171	1.1698	0.9990	
3	13	5	14.698		14.486	14.413	1.593	0.212	1.5909	0.9980	
3	1	6	34.750		34.294	34.438	2.390	0.456	4.7520	0.9869	
3	2	6	27.801		27.859	27.981	0.427	-0.058	-0.5894	0.9911	
3	3	6	8.254		8.193	8.164	0.717	0.061	0.4411	0.9992	
3	4	6	15.263		15.188	15.207	-0.168	0.074	0.6714	0.9974	
3	5	6	42.924		43.392	43.672	3.543	-0.468	-4.6363	0.9807	
3	6	6	2.554		1.525	1.480	0.368	1.029	3.1481	1.0000	
3	7	6	2.643		1.408	-1.383	-0.267	1.235	3.8734	1.0000	
3	8	6	20.630		20.361	-20.390	-0.684	0.269	2.3715	0.9961	
3	9	6	46.202		46.220	46.538	3.637	-0.018	-0.1642	0.9804	
3	10	6	0.963	*	0.408	-0.150	0.379	0.556	0.5856	1.0000	* **
3	11	6	4.505		4.385	4.385	-0.082	0.120	0.5202	0.9998	
3	12	6	4.936		4.282	4.279	-0.188	0.654	2.9711	0.9998	
3	0	7	19.862		18.960	18.992	-0.190	0.902	8.5846	0.9965	
3	1	7	17.506		17.041	16.947	2.007	0.464	4.3061	0.9972	
3	2	7	6.851		6.729	6.706	0.573	0.122	0.8029	0.9995	
3	3	7	27.432		26.566	-26.603	-1.725	0.866	8.1785	0.9930	
3	4	7	23.972		23.097	-23.154	-0.481	0.875	8.0253	0.9947	
3	5	7	17.384		17.051	17.028	1.256	0.333	2.9425	0.9973	
3	6	7	5.593		4.857	-4.857	0.088	0.737	4.1022	0.9998	
3	7	7	8.067		8.065	-8.060	-0.346	0.002	0.0162	0.9994	
3	8	7	2.292		1.129	1.129	0.028	1.162	3.0035	1.0000	
3	9	7	2.154		1.423	-1.419	-0.097	0.732	1.7784	1.0000	
3	10	7	11.103		10.625	10.630	0.107	0.478	3.4610	0.9990	
3	1	8	16.609		15.524	15.485	1.312	1.085	9.5639	0.9978	
3	2	8	23.586		21.814	-21.859	-0.378	1.772	15.9957	0.9956	
3	3	8	38.367		36.263	36.379	2.721	2.104	19.4013	0.9881	
3	4	8	8.545		8.347	-8.348	0.159	0.198	1.3521	0.9994	
3	5	8	5.076		4.148	4.146	0.143	0.928	4.7579	0.9999	
3	6	8	0.387	*	1.399	-1.365	-0.310	-1.012	-0.4489	1.0000	* **
3	7	8	36.507		34.944	34.972	3.294	1.563	13.8256	0.9896	
3	8	8	14.175		13.097	13.093	0.601	1.078	8.4048	0.9986	
3	0	9	2.957		0.779	-0.713	0.313	2.178	8.0390	1.0000	

RFINE 108206 CYCLE 4

STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	1	9	21.109		19.511	-19.468	-1.703	1.598	13.8865	0.9968	
3	2	9	9.016		8.140	-8.132	-0.396	0.876	6.1511	0.9994	
3	3	9	21.630		19.875	19.847	1.568	1.754	15.0838	0.9966	
3	4	9	12.584		11.402	11.398	0.497	1.181	9.1598	0.9989	
4	0	0	100.033		100.513	111.678	4.693	-0.480	-3.6943	0.8086	
4	1	0	15.286		15.616	15.631	0.894	-0.331	-2.1684	0.9949	
4	2	0	4.423		3.431	3.430	-0.100	0.992	3.3323	0.9998	
4	3	0	15.382		14.968	14.997	-0.415	0.414	2.6121	0.9953	
4	4	0	63.795		60.013	62.128	3.932	3.781	26.2386	0.9294	
4	5	0	28.632		28.843	29.050	0.540	-0.211	-1.4375	0.9855	
4	6	0	25.927		25.017	25.119	1.133	0.910	6.0563	0.9899	
4	7	0	22.254		22.560	-22.643	-0.401	-0.306	-1.9533	0.9924	
4	8	0	23.700		23.912	23.922	2.034	-0.213	-1.3212	0.9920	
4	9	0	13.334		13.366	-13.380	-0.244	-0.033	-0.1784	0.9977	
4	10	0	25.136		24.809	24.787	2.412	0.327	1.9367	0.9924	
4	11	0	14.840		15.098	15.113	0.399	-0.258	-1.3479	0.9973	
4	12	0	8.991		8.670	8.669	0.293	0.321	1.3235	0.9991	
4	13	0	1.813	*	1.016	-0.971	-0.300	0.797	0.8792	1.0000	* **
4	14	0	33.036		33.134	33.183	3.144	-0.098	-0.5234	0.9882	
4	1	1	6.732		7.089	7.092	0.050	-0.357	-2.2883	0.9990	
4	2	1	14.449		14.018	14.013	0.961	0.431	3.8184	0.9960	
4	3	1	1.085	*	1.422	1.372	0.371	-0.337	-0.3891	1.0000	* **
4	4	1	22.035		21.614	-21.655	-1.597	0.421	3.7925	0.9908	
4	5	1	31.748		31.326	-31.582	-0.839	0.423	4.0366	0.9831	
4	6	1	37.569		37.668	38.041	2.139	-0.100	-0.9494	0.9774	
4	7	1	3.534		2.559	2.485	0.612	0.974	3.5977	0.9999	
4	8	1	28.474		28.319	-28.386	-2.275	0.156	1.3946	0.9889	
4	9	1	7.796		7.466	7.449	-0.535	0.330	1.9816	0.9993	
4	10	1	29.026		29.018	29.096	2.054	0.009	0.0725	0.9897	
4	11	1	23.413		23.447	23.509	0.814	-0.034	-0.2710	0.9935	
4	12	1	18.452		18.299	-18.274	-1.481	0.153	1.1380	0.9962	
4	13	1	1.707	*	2.384	-2.353	-0.383	-0.677	-0.9997	0.9999	* **
4	14	1	5.123		5.123	5.040	0.927	-0.001	-0.0027	0.9997	
4	0	2	2.572		0.367	-0.315	-0.188	2.205	7.3247	1.0000	
4	1	2	36.662		37.788	-38.255	-0.928	-1.125	-12.2343	0.9751	
4	2	2	63.166		63.404	65.564	4.400	-0.238	-2.5541	0.9310	
4	3	2	15.938		16.051	-16.083	0.405	-0.113	-1.0266	0.9954	
4	4	2	3.746		2.572	2.551	0.331	1.174	4.5177	0.9999	
4	5	2	6.331		5.871	-5.853	-0.471	0.461	2.8112	0.9995	
4	6	2	55.390		56.063	57.282	2.970	-0.673	-6.6403	0.9553	
4	7	2	6.921		6.443	6.435	0.358	0.478	3.0649	0.9994	
4	8	2	27.391		28.127	28.214	1.791	-0.736	-6.6987	0.9899	
4	9	2	9.202		9.008	9.009	0.235	0.194	1.2971	0.9990	
4	10	2	13.692		13.959	13.930	1.120	-0.267	-2.0298	0.9978	
4	11	2	1.470	*	0.570	-0.461	-0.335	0.900	1.2880	1.0000	* **
4	12	2	39.785		40.166	40.409	2.942	-0.381	-3.1303	0.9828	
4	13	2	7.059		6.834	-6.830	0.274	0.224	1.1625	0.9995	
4	14	2	2.891		1.146	-1.122	-0.232	1.746	4.5031	1.0000	
4	1	3	12.193		12.500	-12.515	-0.013	-0.307	-2.8008	0.9976	
4	2	3	20.070		20.692	-20.739	-0.921	-0.622	-6.1492	0.9935	
4	3	3	10.818		11.205	11.212	-0.277	-0.388	-3.2221	0.9981	
4	4	3	26.252		26.646	26.742	1.598	-0.393	-3.8041	0.9892	
4	5	3	23.903		24.608	24.695	0.844	-0.705	-6.7915	0.9918	

RFINE 108206 CYCLE 4

STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
4	6	3	30.396	31.325	-31.459	-1.986	-0.929	-8.9921	0.9875	
4	7	3	6.913	7.267	-7.248	-0.559	-0.354	-2.2530	0.9994	
4	8	3	20.017	20.496	20.423	2.248	-0.479	-4.2350	0.9952	
4	9	3	1.629 *	1.780	1.683	0.582	-0.152	-0.2671	1.0000	* **
4	10	3	20.418	21.235	-21.204	-1.865	-0.817	-6.8031	0.9932	
4	11	3	22.404	22.755	-22.803	-0.750	-0.351	-2.8810	0.9947	
4	12	3	19.066	19.672	19.651	1.531	-0.606	-4.7048	0.9961	
4	13	3	1.780 *	1.650	-1.603	0.388	0.131	0.2210	1.0000	* **
4	0	4	73.290	75.735	78.532	4.326	-2.445	-26.2744	0.9272	
4	1	4	17.313	17.552	17.568	0.839	-0.239	-2.3594	0.9959	
4	2	4	4.426	4.148	4.148	-0.079	0.277	1.4291	0.9998	
4	3	4	12.517	12.331	12.338	-0.380	0.186	1.6135	0.9980	
4	4	4	49.796	50.440	51.125	3.644	-0.644	-6.3481	0.9685	
4	5	4	17.303	18.071	18.100	0.488	-0.768	-7.0070	0.9961	
4	6	4	16.795	16.737	16.731	1.044	0.058	0.5206	0.9968	
4	7	4	14.537	14.935	-14.949	-0.360	-0.398	-3.4044	0.9976	
4	8	4	20.436	20.779	20.740	1.889	-0.342	-3.0061	0.9955	
4	9	4	10.187	10.242	-10.245	-0.222	-0.055	-0.3999	0.9989	
4	10	4	22.502	22.770	22.718	2.241	-0.268	-2.2782	0.9949	
4	11	4	9.447	9.769	9.767	0.361	-0.322	-2.1301	0.9991	
4	12	4	5.396	5.291	5.284	0.270	0.106	0.4902	0.9997	
4	13	4	0.757 *	0.738	0.689	-0.265	0.019	0.0139	1.0000	* **
4	1	5	3.488	3.158	3.157	0.083	0.330	1.4389	0.9999	
4	2	5	5.928	5.865	5.802	0.861	0.063	0.3990	0.9996	
4	3	5	8.029	8.275	8.269	0.395	-0.246	-1.7312	0.9992	
4	4	5	10.476	10.375	-10.291	-1.360	0.102	0.7937	0.9988	
4	5	5	24.487	24.449	-24.516	-0.709	0.038	0.3495	0.9937	
4	6	5	28.324	28.865	28.923	1.959	-0.541	-5.0440	0.9915	
4	7	5	1.293 *	1.303	-1.171	0.572	-0.010	-0.0145	1.0000	* **
4	8	5	24.166	24.659	-24.653	-1.957	-0.492	-4.3457	0.9942	
4	9	5	10.657	10.743	10.741	-0.416	-0.086	-0.6389	0.9989	
4	10	5	26.027	26.364	26.379	1.918	-0.3[illegible]	-2.8803	0.9936	
4	11	5	16.765	17.293	17.300	0.757	-0.528	-4.1105	0.9973	
4	12	5	12.662	12.712	-12.663	-1.213	-0.050	-0.3582	0.9985	
4	0	6	4.831	5.104	-5.102	-0.162	-0.273	-1.4811	0.9997	
4	1	6	17.943	17.779	-17.792	-0.773	0.164	1.5083	0.9967	
4	2	6	45.592	44.532	44.836	3.772	1.060	10.2785	0.9795	
4	3	6	10.277	9.828	-9.827	0.345	0.449	3.4135	0.9990	
4	4	6	4.833	4.579	4.569	0.306	0.254	1.2356	0.9998	
4	5	6	9.721	9.667	-9.663	-0.419	0.053	0.3897	0.9991	
4	6	6	33.011	33.396	33.476	2.526	-0.386	-3.5218	0.9896	
4	7	6	8.857	8.799	8.796	0.328	0.058	0.4014	0.9993	
4	8	6	21.108	21.276	21.264	1.547	-0.169	-1.4384	0.9959	
4	9	6	6.932	6.902	6.900	0.211	0.031	0.1814	0.9996	
4	10	6	12.518	12.841	12.813	0.982	-0.323	-2.3771	0.9986	
4	1	7	8.507	8.119	-8.122	0.023	0.388	2.7047	0.9994	
4	2	7	14.429	13.992	-13.985	-0.742	0.437	3.5578	0.9982	
4	3	7	9.481	9.126	9.128	-0.176	0.354	2.5304	0.9992	
4	4	7	18.965	18.201	18.179	1.349	0.763	6.5003	0.9970	
4	5	7	14.915	14.717	14.713	0.733	0.198	1.6029	0.9981	
4	6	7	19.536	19.125	-19.091	-1.569	0.411	3.4880	0.9968	
4	7	7	6.222	6.016	-6.002	-0.422	0.206	1.1690	0.9997	
4	8	7	13.169	13.076	12.946	1.905	0.093	0.7042	0.9985	

RFINE 108206 CYCLE 4

STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTCR	
4	0	8	42.197		39.869	40.006	3.399	2.328	21.0858	0.9861	
4	1	8	16.181		15.174	15.175	0.683	1.006	8.2437	0.9980	
4	2	8	4.635		4.498	4.498	-0.036	0.137	0.6187	0.9998	
4	3	8	7.185		6.794	6.789	-0.291	0.391	2.3152	0.9996	
4	4	8	35.259		33.258	33.299	2.897	2.001	17.3095	0.9900	
4	5	8	5.341		5.434	5.423	0.367	-0.094	-0.4636	0.9998	
5	1	0	28.244		27.456	27.571	1.786	0.788	5.0910	0.9876	
5	2	0	16.320		15.814	-15.839	-0.494	0.506	7.9216	0.9959	
5	3	0	55.156		54.217	55.450	3.265	0.938	6.0108	0.9527	
5	4	0	11.858		12.321	12.325	0.533	-0.463	-2.2590	0.9975	
5	5	0	14.721		14.288	-14.309	0.040	0.432	2.0877	0.9971	
5	6	0	2.889		2.690	-2.595	-0.707	0.199	0.3964	0.9999	
5	7	0	41.369		41.833	42.128	3.862	-0.463	-2.8421	0.9778	
5	8	0	14.183		14.209	14.192	0.990	-0.026	-0.1340	0.9976	
5	9	0	18.603		18.633	18.671	-0.100	-0.030	-0.1620	0.9960	
5	10	0	3.943		5.331	-5.283	-0.719	-1.388	-2.9158	0.9997	
5	11	0	49.010		49.214	49.744	3.440	-0.204	-1.1650	0.9741	
5	12	0	3.040		2.472	2.422	0.495	0.569	1.0670	0.9999	
5	13	0	5.511		3.193	3.175	0.348	2.318	6.8045	0.9999	
5	0	1	4.883		1.152	0.865	0.761	3.731	18.0122	1.0000	
5	1	1	40.139		40.423	-40.890	-2.303	-0.284	-2.6630	0.9742	
5	2	1	17.041		16.990	-17.006	-0.901	0.051	0.4348	0.9954	
5	3	1	8.836		7.335	7.137	1.706	1.501	9.8617	0.9991	
5	4	1	16.107		15.051	15.058	0.793	1.056	8.2522	0.9964	
5	5	1	28.430		28.064	-28.192	-1.306	0.365	3.1689	0.9889	
5	6	1	2.434		0.442	0.375	-0.233	1.993	4.8146	1.0000	
5	7	1	15.561		15.051	15.059	0.651	0.509	3.8814	0.9971	
5	8	1	0.639	*	1.906	1.904	0.074	-1.267	-0.7700	1.0000	* **
5	9	1	11.205		10.922	10.922	0.416	0.283	1.8818	0.9986	
5	10	1	1.527	*	0.523	0.509	0.119	1.004	1.4390	1.0000	* **
5	11	1	14.181		14.069	-14.051	-0.966	0.111	0.7581	0.9979	
5	12	1	6.483		5.753	-5.729	-0.532	0.730	3.4445	0.9997	
5	13	1	10.883		10.903	10.832	1.306	-0.020	-0.1230	0.9988	
5	1	2	24.266		25.543	25.556	2.347	-1.278	-11.9675	0.9907	
5	2	2	5.793		5.021	5.001	0.459	0.772	4.2195	0.9996	
5	3	2	30.934		31.427	31.640	0.925	-0.493	-4.4648	0.9857	
5	4	2	2.220		3.047	-3.007	-0.492	-0.827	-1.8289	0.9999	
5	5	2	60.398		60.605	61.933	3.859	-0.208	-1.9030	0.9539	
5	6	2	4.803		4.354	4.297	0.705	0.449	2.0468	0.9998	
5	7	2	1.826	*	1.964	-1.962	-0.100	-0.138	-0.2421	1.0000	* **
5	8	2	21.301		21.569	-21.603	-0.989	-0.268	-2.2086	0.9948	
5	9	2	40.577		41.839	42.080	3.628	-1.262	-10.7356	0.9813	
5	10	2	10.044		10.326	10.306	0.733	-0.282	-1.8081	0.9989	
5	11	2	14.061		13.771	-13.783	-0.198	0.290	2.0614	0.9981	
5	12	2	1.478	*	0.465	0.009	-0.465	1.012	1.3700	1.0000	* **
5	0	3	4.899		5.037	-4.991	-0.685	-0.138	-0.7232	0.9997	
5	1	3	43.890		45.461	46.016	2.251	-1.571	-15.1686	0.9737	
5	2	3	17.747		18.452	18.469	0.933	-0.705	-6.2441	0.9956	
5	3	3	5.568		5.546	-5.310	-1.604	0.022	0.1187	0.9996	
5	4	3	10.240		9.924	-9.906	-0.695	0.316	2.2697	0.9987	
5	5	3	16.435		17.161	17.142	1.280	-0.726	-5.9760	0.9966	
5	6	3	4.193		4.005	-3.997	0.265	0.187	0.7563	0.9998	
5	7	3	6.330		5.876	-5.853	-0.533	0.454	2.4756	0.9996	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
5	8	3	1.406 *	0.132	0.131	-0.014	1.274	1.8121	1.0000	* **
5	9	3	8.007	7.319	-7.314	-0.310	0.688	4.2218	0.9995	
5	10	3	3.139	2.498	2.497	-0.055	0.641	1.9435	0.9999	
5	11	3	8.010	7.535	7.471	0.998	0.475	2.8403	0.9995	
5	12	3	3.554	2.892	2.840	0.545	0.662	2.1760	0.9999	
5	1	4	24.915	24.884	24.917	1.665	0.032	0.2947	0.9929	
5	2	4	11.000	10.890	-10.888	-0.451	0.110	0.8216	0.9986	
5	3	4	39.036	39.768	40.027	3.007	-0.732	-6.6987	0.9815	
5	4	4	7.535	8.065	8.054	0.486	-0.531	-3.3760	0.9992	
5	5	4	9.470	9.658	-9.662	0.050	-0.188	-1.3209	0.9990	
5	6	4	3.097	2.594	-2.511	-0.651	0.503	1.5946	0.9999	
5	7	4	36.365	37.775	37.873	3.581	-1.410	-12.4438	0.9860	
5	8	4	13.191	13.547	13.527	0.924	-0.356	-2.6527	0.9982	
5	9	4	12.041	12.098	12.106	-0.096	-0.057	-0.4072	0.9986	
5	10	4	5.050	5.795	-5.758	-0.665	-0.745	-3.2255	0.9997	
5	11	4	42.746	43.535	43.798	3.188	-0.789	-6.5546	0.9828	
5	0	5	1.677 *	2.112	-1.987	0.718	-0.435	-0.5236	1.0000	* **
5	1	5	23.830	24.002	-23.991	-2.013	-0.172	-1.5415	0.9939	
5	2	5	10.322	10.387	-10.367	-0.739	-0.065	-0.4882	0.9989	
5	3	5	6.454	6.725	6.547	1.543	-0.271	-1.5234	0.9995	
5	4	5	13.932	13.781	13.774	0.766	0.151	1.1648	0.9930	
5	5	5	25.713	26.138	-26.200	-1.129	-0.425	-3.5870	0.9934	
5	6	5	1.794 *	2.080	-2.073	-0.162	-0.286	-0.5317	1.0000	* **
5	7	5	16.680	16.447	16.455	0.660	0.233	1.8696	0.9975	
5	8	5	3.126	2.865	2.862	0.117	0.261	0.8256	0.9999	
5	9	5	10.314	10.311	10.306	0.452	0.003	0.0176	0.9991	
5	10	5	3.342	3.001	2.997	0.155	0.341	1.1063	0.9999	
5	1	6	21.243	21.370	21.321	2.024	-0.127	-1.0925	0.9956	
5	2	6	7.250	6.372	6.360	0.406	0.878	5.3640	0.9996	
5	3	6	14.886	14.857	14.853	0.779	0.029	0.2209	0.9979	
5	4	6	4.270	4.763	-4.744	-0.424	-0.493	-1.9985	0.9998	
5	5	6	46.676	45.547	45.856	3.314	1.129	9.9814	0.9814	
5	6	6	3.127	2.979	2.918	0.601	0.148	0.4610	0.9999	
5	7	6	1.159 *	1.943	1.942	-0.055	-0.784	-0.9365	1.0000	* **
5	8	6	12.293	12.843	-12.825	-0.832	-0.550	-3.9753	0.9986	
5	0	7	4.908	4.204	-4.174	-0.510	0.704	3.4057	0.9998	
5	1	7	32.753	31.372	31.458	1.860	1.381	11.9316	0.9910	
5	2	7	13.338	12.934	12.918	0.817	0.405	3.0799	0.9985	
5	3	7	2.943	3.924	-3.709	-1.282	-0.981	-2.8304	0.9999	
5	4	7	5.134	5.027	-5.001	-0.521	0.107	0.4925	0.9998	
5	5	7	10.915	9.859	9.804	1.084	1.056	7.6195	0.9992	
6	0	0	26.531	26.464	26.329	3.762	0.067	0.3742	0.9901	
6	1	0	24.996	25.214	25.304	1.078	-0.218	-1.2112	0.9910	
6	2	0	5.615	5.867	-5.869	-0.002	-0.252	-0.7480	0.9995	
6	3	0	6.179	6.769	-6.727	-0.777	-0.590	-1.8728	0.9994	
6	4	0	59.489	57.969	59.197	3.526	1.520	8.7012	0.9555	
6	5	0	6.008	6.493	-6.471	0.554	-0.485	-1.5334	0.9995	
6	6	0	29.032	29.568	29.698	1.225	-0.536	-2.9367	0.9896	
6	7	0	5.682	5.670	-5.663	-0.309	0.012	0.0361	0.9996	
6	8	0	22.688	23.269	23.269	1.812	-0.582	-3.0593	0.9940	
6	9	0	5.749	5.734	-5.733	-0.156	0.015	0.0429	0.9996	
6	10	0	12.503	13.456	13.321	1.987	-0.953	-4.2403	0.9981	
6	11	0	2.387 *	1.211	-1.142	0.403	1.176	1.6611	1.0000	* **

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
6	1	1	11.539	11.500	11.510	-0.074	0.040	0.2681	0.9982	
6	2	1	29.771	29.263	29.420	0.970	0.507	4.1110	0.9883	
6	3	1	5.695	6.131	6.109	0.532	-0.436	-1.8440	0.9995	
6	4	1	3.774	4.241	-4.068	-1.201	-0.467	-1.4130	0.9998	
6	5	1	15.325	14.946	-14.942	-0.852	0.379	2.6677	0.9973	
6	6	1	11.936	11.890	11.783	1.666	0.046	0.2988	0.9983	
6	7	1	6.663	6.493	6.433	0.887	0.170	0.8311	0.9995	
6	8	1	37.983	37.834	-38.078	-2.049	0.149	1.1582	0.9844	
6	9	1	12.400	12.447	-12.428	-0.861	-0.047	-0.3099	0.9983	
6	10	1	12.250	12.393	12.296	1.623	-0.143	-0.9049	0.9984	
6	0	2	21.283	22.162	22.229	0.134	-0.879	-7.1784	0.9939	
6	1	2	6.956	6.908	-6.838	-0.999	0.047	0.2632	0.9994	
6	2	2	56.126	57.723	58.806	3.861	-1.597	-13.6566	0.9594	
6	3	2	7.287	8.073	8.040	0.770	-0.786	-4.1988	0.9992	
6	4	2	6.280	5.208	-5.200	0.306	1.071	5.2643	0.9997	
6	5	2	10.701	10.734	-10.724	-0.594	-0.033	-0.2127	0.9987	
6	6	2	12.265	12.601	12.386	2.380	-0.336	-2.2730	0.9983	
6	7	2	18.018	18.345	18.375	0.358	-0.327	-2.4287	0.9964	
6	8	2	18.410	18.651	18.615	1.611	-0.241	-1.7892	0.9964	
6	9	2	9.315	9.132	9.134	0.177	0.183	1.0912	0.9992	
6	10	2	25.016	24.781	24.828	1.192	0.235	1.7874	0.9939	
6	1	3	4.940	4.560	-4.558	0.155	0.380	1.7167	0.9998	
6	2	3	23.768	24.395	-24.462	-0.905	-0.627	-5.1796	0.9932	
6	3	3	13.618	13.974	-13.982	-0.476	-0.356	-2.5187	0.9978	
6	4	3	3.617	3.052	2.812	1.188	0.565	1.9698	0.9999	
6	5	3	17.896	17.915	17.923	0.896	-0.020	-0.1518	0.9966	
6	6	3	10.611	10.770	-10.665	-1.544	-0.159	-1.0560	0.9988	
6	7	3	1.452 *	0.798	-0.202	-0.772	0.653	0.9001	1.0000	* **
6	8	3	36.497	37.408	37.607	2.048	-0.911	-7.3999	0.9865	
6	9	3	4.777	5.220	5.150	0.857	-0.444	-1.7622	0.9997	
6	0	4	22.892	23.769	23.585	3.482	-0.877	-7.2605	0.9940	
6	1	4	16.657	17.348	17.348	0.982	-0.690	-5.4052	0.9968	
6	2	4	5.011	5.162	-5.162	0.004	-0.150	-0.6613	0.9997	
6	3	4	5.590	6.113	-6.072	-0.716	-0.523	-2.4573	0.9996	
6	4	4	48.355	48.669	49.147	3.262	-0.314	-2.6549	0.9763	
6	5	4	3.059	1.874	-1.799	0.527	1.184	3.7019	1.0000	
6	6	4	25.060	25.680	25.736	1.143	-0.620	-4.9977	0.9937	
6	7	4	7.009	7.596	-7.593	-0.295	-0.587	-3.0666	0.9995	
6	8	4	18.912	19.982	19.949	1.679	-1.070	-8.1264	0.9963	
6	1	5	12.483	12.597	12.607	0.010	-0.114	-0.8419	0.9984	
6	2	5	23.996	23.634	23.683	0.886	0.363	2.9769	0.9944	
6	3	5	1.426 *	0.668	-0.429	0.512	0.758	1.0629	1.0000	* **
6	4	5	4.843	4.507	-4.388	-1.030	0.336	1.5250	0.9998	
6	5	5	8.381	8.666	-8.642	-0.688	-0.285	-1.7172	0.9993	
6	6	5	10.086	10.216	10.106	1.530	-0.130	-0.8659	0.9990	
6	7	5	9.188	9.432	9.397	0.857	-0.244	-1.5298	0.9992	
6	0	6	16.700	16.549	16.569	0.178	0.151	1.1410	0.9974	
6	1	6	10.583	10.315	-10.283	-0.872	0.268	1.7755	0.9990	
6	2	6	42.346	41.774	41.992	3.302	0.572	4.7586	0.9835	
6	3	6	6.486	5.920	5.885	0.656	0.566	3.0255	0.9997	
6	4	6	4.300	3.937	-3.928	0.270	0.363	1.4157	0.9999	
7	1	0	39.114	37.343	37.645	1.704	1.771	9.2175	0.9820	
7	2	0	8.180	8.494	-8.490	-0.389	-0.314	-1.0997	0.9991	

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
7	3	0	23.911		23.770	23.706	2.688	0.141	0.6879	0.9926	
7	4	0	6.023		4.595	4.539	0.717	1.429	4.3412	0.9997	
7	5	0	2.154	*	1.814	-1.808	0.147	0.339	0.4251	1.0000	* **
7	6	0	9.235		9.373	-9.332	-0.922	-0.138	-0.5261	0.9990	
7	7	0	33.868		34.204	34.275	3.189	-0.336	-1.7211	0.9873	
7	0	1	8.373		8.566	8.500	1.092	-0.193	-0.9669	0.9991	
7	1	1	27.262		26.555	-26.609	-1.859	0.707	5.0924	0.9911	
7	2	1	12.151		12.366	-12.340	-0.972	-0.215	-1.2682	0.9980	
7	3	1	9.205		9.587	9.505	1.295	-0.381	-1.9973	0.9988	
7	4	1	11.556		11.479	11.460	0.788	0.078	0.4686	0.9985	
7	5	1	6.009		5.570	-5.483	-0.989	0.438	1.8449	0.9996	
7	6	1	2.141	*	1.220	-1.142	-0.428	0.921	1.6208	1.0000	* **
7	7	1	14.876		14.884	14.890	0.585	-0.008	-0.0501	0.9976	
7	1	2	15.340		15.572	15.470	1.958	-0.231	-1.5730	0.9972	
7	2	2	7.672		8.278	8.273	0.385	-0.606	-3.0364	0.9992	
7	3	2	4.093		2.418	2.268	0.840	1.674	5.4827	0.9999	
7	4	2	5.327		4.321	-4.265	-0.696	1.006	4.2079	0.9998	
7	5	2	45.804		46.377	46.790	3.293	-0.573	-4.4230	0.9776	
7	6	2	8.545		8.937	8.894	0.911	-0.392	-2.2353	0.9992	
7	7	2	12.131		12.331	12.340	0.153	-0.200	-1.2555	0.9985	
7	0	3	6.848		7.144	-7.079	-0.976	-0.296	-1.4579	0.9994	
7	1	3	17.354		17.874	17.818	1.771	-0.520	-3.6574	0.9965	
7	2	3	11.891		12.374	12.344	1.007	-0.483	-3.0456	0.9983	
7	3	3	8.671		9.368	-9.294	-1.217	-0.697	-3.9931	0.9990	
7	4	3	9.400		9.913	-9.894	-0.685	-0.513	-3.0431	0.9990	
7	5	3	12.427		12.511	12.479	1.023	-0.084	-0.5412	0.9984	
7	6	3	3.128		1.886	1.824	0.480	1.242	3.6882	1.0000	
7	1	4	29.739		30.125	30.227	1.575	-0.386	-2.9610	0.9906	
7	2	4	6.864		7.286	-7.279	-0.358	-0.422	-2.0834	0.9995	
7	3	4	23.861		24.365	24.310	2.503	-0.504	-3.7661	0.9939	
7	4	4	4.962		4.025	3.970	0.663	0.938	3.8639	0.9998	

RFINE 108206 CYCLE 4

RESULTS OF STRUCTURE FACTOR CALCULATION

	NUMERATOR	DENOMINATOR	NUMBER	R
ALL REFLECTIONS				
WEIGHTED R	156674.38	65553232.00	773	0.049
UNWEIGHTED R	587.42	15283.48	773	0.038
RANGES OF F(OBS)				
	6344.80	38585664.00	455	0.013
	14001.61	15688674.00	185	0.030
	17716.83	6529880.00	77	0.052
	45511.65	2883324.00	34	0.126
	8211.89	1102447.00	13	0.086
	17267.14	339214.38	4	0.226
	36589.86	339214.38	4	0.328
	11050.32	84803.63	1	0.361
RANGES OF (SIN(THETA)/LAMBDA)**2				
	95609.88	3816164.00	45	0.158
	31336.91	5512238.00	65	0.075
	8449.83	7038701.00	83	0.035
	5527.70	8310758.00	98	0.026
	3398.41	8734776.00	103	0.020
	3364.59	10261240.00	121	0.018
	3172.73	10346043.00	122	0.018
	5833.98	11533297.00	136	0.022
UNREJECTED REFLECTIONS				
WEIGHTED R	156592.19	65553184.00	723	0.049
UNWEIGHTED R	551.21	15211.66	723	0.036
RANGES OF F(OBS)				
	6261.72	36720656.00	405	0.013
	14001.61	16773635.00	185	0.029
	17716.83	6981459.00	77	0.050
	45511.65	3082722.00	34	0.122
	8211.89	1178687.00	13	0.083
	17267.14	362673.19	4	0.218
	36589.86	362673.19	4	0.318
	11050.32	90668.25	1	0.349
RANGES OF (SIN(THETA)/LAMBDA)**2				
	95595.63	3717400.00	41	0.160
	31336.42	5802771.00	64	0.073
	8431.53	6981459.00	77	0.035
	5522.16	8522820.00	94	0.025
	3385.17	8794824.00	97	0.020
	3354.00	9973512.00	110	0.018
	3168.22	10426854.00	115	0.017
	5817.84	11333537.00	125	0.023

SUM FCAL 15119.30

STANDARD DEV OF UNIT WEIGHT OBS 15.14

RFINE 108206 CYCLE 4

ATOM	PARAMETER	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR	
ESTIMATED STD. DEV. FOR OBS. OF UNIT WEIGHT		15.14					
EXTINCTION CORRECTION ISOTROPIC	R-STAR	0.1738E 00		0.1738E 00			
	SCALE FACTOR 1	9.2610		9.2610			
ATOM 1 M1	EQUIPOINT FRACTION = 0.500						
	OCCUPANCY SPECIES 1	0.17191	0.00000	0.17191	0.00852	0.00	1
	OCCUPANCY SPECIES 2	0.82809		0.82809			
	TOTAL OCCUPANCY (FIXED) =	1.00000					
	X	0.0		0.0			
	Y	0.0		0.0			
	Z	0.0		0.0			
	BETA11	0.0057800	-0.0000000	0.0057799	0.0004221	-0.00	2
	BETA22	0.0021662	-0.0000000	0.0021662	0.0000975	-0.00	3
	BETA33	0.0047871	-0.0000000	0.0047871	0.0002338	-0.00	4
	BETA12	-0.0000283	0.0000000	-0.0000283	0.0001858	0.00	5
	BETA13	-0.0007489	-0.0000000	-0.0007489	0.0002667	-0.00	6
	BETA23	-0.0006874	0.0000000	-0.0006874	0.0001046	0.00	7
ATOM 2 M2	EQUIPOINT FRACTION = 0.500						
	OCCUPANCY SPECIES 1	0.00809		0.00809			
	OCCUPANCY SPECIES 2	0.99191		0.99191			
	TOTAL OCCUPANCY (FIXED) =	1.00000					
	X	0.9876623	-0.0000001	0.9876621	0.0002444	-0.00	8
	Y	0.2801470	0.0000000	0.2801470	0.0000980	0.00	9
	Z	0.2500000		0.2500000			
	BETA11	0.0066843	-0.0000001	0.0066842	0.0003705	-0.00	10
	BETA22	0.0013702	-0.0000000	0.0013702	0.0000707	-0.00	11
	BETA33	0.0050082	-0.0000001	0.0050081	0.0001773	-0.00	12
	BETA12	0.0001222	-0.0000000	0.0001222	0.0001614	-0.00	13
	BETA13	0.0		0.0			
	BETA23	0.0		0.0			
ATOM 3 SI	EQUIPOINT FRACTION = 0.500						
	OCCUPANCY SPECIES 3	1.00000		1.00000			
	X	0.4265044	-0.0000001	0.4265043	0.0004186	-0.00	14
	Y	0.0951376	0.0000000	0.0951376	0.0001943	0.00	15
	Z	0.2500000		0.2500000			
	BETA11	0.0054112	0.0000001	0.0054113	0.0006759	0.00	16
	BETA22	0.0014092	-0.0000000	0.0014092	0.0001386	-0.00	17
	BETA33	0.0044723	-0.0000000	0.0044723	0.0003488	-0.00	18
	BETA12	0.0000896	0.0000000	0.0000897	0.0002640	0.00	19
	BETA13	0.0		0.0			
	BETA23	0.0		0.0			
ATOM 4 O1	EQUIPOINT FRACTION = 0.500						
	OCCUPANCY SPECIES 4	1.00000		1.00000			
	X	0.7573454	0.0000001	0.7573455	0.0010419	0.00	20
	Y	0.0914241	-0.0000000	0.0914240	0.0005161	-0.00	21
	Z	0.2500000		0.2500000			
	BETA11	0.0029444	-0.0000001	0.0029442	0.0017574	-0.00	22
	BETA22	0.0024576	0.0000000	0.0024576	0.0004258	0.00	23
	BETA33	0.0066857	0.0000001	0.0066859	0.0010018	0.00	24
	BETA12	0.0000627	-0.0000000	0.0000627	0.0007686	-0.00	25
	BETA13	0.0		0.0			
	BETA23	0.0		0.0			

ATOM 5 O2	EQUIPOINT FRACTION = 0.500						
	OCCUPANCY SPECIES 4	1.00000		1.00000			
	X	0.2161920	-0.0000001	0.2161918	0.0010731	-0.00	26
	Y	0.4524900	0.0000001	0.4524900	0.0004696	0.00	27
	Z	0.2500000		0.2500000			
	BETA11	0.0057160	-0.0000001	0.0057159	0.0018198	-0.00	28
	BETA22	0.0014470	0.0000000	0.0014470	0.0003807	0.00	29
	BETA33	0.0056397	0.0000000	0.0056397	0.0009196	0.00	30
	BETA12	-0.0001527	-0.0000000	-0.0001528	0.0007079	-0.00	31
	BETA13	0.0		0.0			
	BETA23	0.0		0.0			
ATOM 6 . O3	EQUIPOINT FRACTION = 1.000						
	OCCUPANCY SPECIES 4	1.00000		1.00000			
	X	0.2856678	0.0000000	0.2856678	0.0007888	0.00	32
	Y	0.1625297	-0.0000000	0.1625296	0.0003293	-0.00	33
	Z	0.0400593	-0.0000000	0.0400593	0.0004964	-0.00	34
	BETA11	0.0075079	0.0000001	0.0075080	0.0013347	0.00	35
	BETA22	0.0018599	0.0000000	0.0018600	0.0002759	0.00	36
	BETA33	0.0049291	0.0000000	0.0049291	0.0006491	0.00	37
	BETA12	0.0001707	0.0000000	0.0001707	0.0005111	0.00	38
	BETA13	0.0000837	0.0000000	0.0000838	0.0007503	0.00	39
	BETA23	0.0003964	0.0000000	0.0003964	0.0003480	0.00	40

MAXIMUM SHIFT/ERROR = -0.00

AVERAGE SHIFT/ERROR = 0.00

RFINE 108206 CYCLE 4

CORRELATION MATRIX

ROW 1

1	1.0000	2	-0.3722	3	-0.4388	4	-0.4804	5	0.0001	6	0.0038	7	0.0193	8	-0.0075	9	-0.0085	10	-0.0174
11	0.0522	12	0.0384	13	0.0027	14	-0.0029	15	-0.0126	16	0.0227	17	-0.0058	18	0.0018	19	0.0189	20	0.0344
21	-0.0414	22	-0.0083	23	0.0030	24	0.0160	25	-0.0018	26	0.0319	27	0.0488	28	0.0053	29	-0.0248	30	0.0176
31	0.0078	32	0.0222	33	-0.0591	34	0.0061	35	0.0243	36	0.0246	37	-0.0124	38	0.0182	39	-0.0059	40	0.0064

ROW 2

2	1.0000	3	-0.0298	4	-0.0042	5	0.0066	6	-0.0217	7	0.0074	8	0.0571	9	0.0061	10	-0.1506	11	0.0376
12	0.0045	13	-0.0029	14	-0.0041	15	0.0190	16	-0.0748	17	0.0139	18	0.0138	19	-0.0187	20	-0.0457	21	0.0127
22	-0.0257	23	0.0129	24	0.0205	25	0.0599	26	0.0067	27	-0.0101	28	-0.0733	29	0.0224	30	-0.0233	31	-0.0252
32	0.0553	33	0.0056	34	0.0050	35	-0.0507	36	-0.0240	37	0.0208	38	-0.0135	39	-0.0359	40	0.0053		

ROW 3

3	1.0000	4	0.0023	5	-0.0041	6	0.0061	7	-0.0572	8	-0.0011	9	0.0017	10	0.0584	11	-0.2063	12	0.0326
13	0.0006	14	-0.0004	15	-0.0190	16	0.0034	17	-0.0261	18	-0.0042	19	-0.0350	20	-0.0050	21	0.0211	22	0.0214
23	0.0100	24	-0.0287	25	-0.0208	26	-0.0220	27	-0.0205	28	0.0069	29	0.0402	30	-0.0137	31	-0.0098	32	-0.0424
33	0.0199	34	0.0120	35	-0.0221	36	-0.0068	37	0.0073	38	-0.0160	39	0.0135	40	-0.0091				

ROW 4

4	1.0000	5	0.0032	6	-0.0270	7	-0.0518	8	0.0077	9	0.0063	10	0.0213	11	0.0260	12	-0.1612	13	-0.0051
14	0.0080	15	0.0131	16	0.0018	17	-0.0000	18	-0.0136	19	-0.0068	20	-0.0165	21	0.0129	22	-0.0080	23	-0.0236
24	0.0324	25	0.0094	26	-0.0090	27	-0.0280	28	-0.0205	29	0.0076	30	0.0282	31	-0.0048	32	-0.0059	33	0.0317
34	-0.0137	35	0.0043	36	-0.0117	37	0.0087	38	0.0020	39	-0.0012	40	0.0121						

ROW 5

5	1.0000	6	-0.0396	7	-0.0192	8	-0.0310	9	0.0168	10	-0.0234	11	0.0006	12	0.0028	13	-0.0447	14	-0.0126
15	0.0267	16	0.0287	17	0.0218	18	-0.0124	19	0.0078	20	0.0105	21	-0.0204	22	-0.0264	23	-0.0360	24	0.0154
25	0.0108	26	-0.0280	27	0.0034	28	-0.0460	29	0.0009	30	0.0153	31	-0.0494	32	0.0340	33	-0.0116	34	-0.0320
35	-0.0118	36	-0.0469	37	0.0131	38	-0.0325	39	-0.0378	40	0.0038								

ROW 6

6	1.0000	7	-0.0017	8	0.0570	9	-0.0054	10	0.0158	11	-0.0019	12	0.0127	13	0.0282	14	0.0213	15	-0.0072
16	-0.0306	17	0.0078	18	-0.0352	19	0.0160	20	0.0152	21	0.0120	22	0.0099	23	0.0044	24	-0.0122	25	0.0011
26	-0.0267	27	0.0155	28	-0.0191	29	0.0026	30	-0.0239	31	-0.0034	32	-0.0078	33	0.0085	34	-0.0007	35	-0.0575
36	0.0081	37	0.0272	38	-0.0378	39	-0.0180	40	-0.0050										

ROW 7

7	1.0000	8	0.0066	9	0.0054	10	-0.0131	11	-0.0066	12	-0.0091	13	0.0025	14	0.0002	15	0.0189	16	-0.0102
17	0.0048	18	-0.0013	19	-0.0059	20	0.0005	21	-0.0031	22	-0.0014	23	-0.0164	24	-0.0151	25	0.0191	26	0.0074
27	-0.0006	28	0.0249	29	-0.0076	30	-0.0009	31	0.0180	32	-0.0065	33	-0.0332	34	0.0019	35	0.0232	36	-0.0410
37	-0.0195	38	-0.0095	39	-0.0093	40	0.0010												

ROW 8

8	1.0000	9	0.0014	10	0.0612	11	0.0226	12	-0.0053	13	0.0203	14	0.0728	15	0.0172	16	-0.0981	17	-0.0413
18	0.0050	19	-0.0229	20	0.0022	21	0.0221	22	0.0827	23	-0.0043	24	-0.0317	25	0.0320	26	0.0524	27	0.0089
28	-0.0327	29	0.0108	30	0.0227	31	-0.0163	32	0.0245	33	-0.0008	34	-0.0261	35	-0.0471	36	-0.0098	37	0.0215
38	-0.0186	39	-0.0159	40	0.0098														

ROW 9

9	1.0000	10	-0.0026	11	0.0042	12	-0.0024	13	-0.0724	14	-0.0077	15	0.0550	16	0.0043	17	-0.0037	18	0.0025
19	0.0514	20	-0.0037	21	0.0087	22	-0.0051	23	-0.0324	24	0.0211	25	0.0156	26	-0.0137	27	0.0236	28	-0.0268
29	-0.0150	30	0.0021	31	-0.0377	32	0.0313	33	0.0106	34	-0.0184	35	-0.0048	36	-0.0062	37	-0.0098	38	0.0132
39	0.0018	40	0.0153																

ROW 10

10	1.0000	11	-0.2330	12	-0.2275	13	0.0200	14	0.0426	15	-0.0183	16	-0.0511	17	0.0058	18	0.0211	19	0.0191
20	0.0490	21	0.0040	22	0.0518	23	-0.0104	24	0.0034	25	-0.0519	26	-0.0351	27	-0.0137	28	0.0275	29	-0.0024
30	-0.0007	31	0.0209	32	-0.0542	33	0.0167	34	0.0004	35	-0.0130	36	0.0089	37	-0.0000	38	-0.0085	39	0.0469
40	-0.0076																		

```
ROW  11
11  1.0000  12 -0.2545  13 -0.0021  14 -0.0035  15  0.0203  16  0.0059  17 -0.0749  18  0.0267  19  0.0359  20 -0.0081
21 -0.0040  22 -0.0112  23 -0.0255  24  0.0115  25  0.0116  26  0.0125  27  0.0244  28 -0.0048  29 -0.0451  30  0.0080
31 -0.0244  32  0.0224  33 -0.0142  34 -0.0097  35  0.0061  36 -0.0116  37  0.0041  38 -0.0102  39 -0.0168  40  0.0042

ROW  12
12  1.0000  13 -0.0009  14  0.0137  15 -0.0010  16  0.0203  17  0.0266  18 -0.0940  19 -0.0126  20  0.0068  21  0.0105
22  0.0052  23  0.0113  24 -0.0298  25  0.0043  26 -0.0005  27  0.0061  28  0.0013  29  0.0051  30 -0.0117  31 -0.0026
32  0.0056  33 -0.0061  34  0.0394  35 -0.0006  36  0.0043  37 -0.0297  38 -0.0094  39  0.0187  40 -0.0095

ROW  13
13  1.0000  14 -0.0033  15 -0.0503  16 -0.0225  17  0.0296  18 -0.0028  19 -0.0014  20  0.0017  21  0.0059  22  0.0111
23  0.0075  24  0.0016  25 -0.0348  26  0.0097  27  0.0093  28  0.0243  29  0.0068  30  0.0126  31  0.0028  32 -0.0138
33 -0.0219  34  0.0040  35  0.0017  36 -0.0079  37 -0.0001  38 -0.0130  39  0.0165  40 -0.0077

ROW  14
14  1.0000  15 -0.0039  16 -0.1026  17  0.0110  18  0.0181  19 -0.0313  20  0.0260  21  0.0120  22  0.0514  23 -0.0182
24 -0.0101  25 -0.0061  26  0.0231  27  0.0066  28  0.0249  29 -0.0018  30 -0.0198  31 -0.0143  32  0.0125  33  0.0000
34  0.0155  35  0.0265  36 -0.0105  37 -0.0196  38  0.0019  39 -0.0483  40  0.0021

ROW  15
15  1.0000  16  0.0042  17 -0.0234  18  0.0099  19 -0.0092  20 -0.0100  21 -0.2351  22  0.0041  23 -0.0443  24  0.0049
25  0.0327  26  0.0123  27  0.0098  28 -0.0262  29  0.0036  30 -0.0005  31  0.0121  32  0.0189  33 -0.0165  34 -0.0006
35  0.0006  36  0.0093  37  0.0013  38 -0.0188  39 -0.0058  40  0.0109

ROW  16
16  1.0000  17 -0.2231  18 -0.2462  19  0.0116  20 -0.0571  21 -0.0190  22 -0.2365  23  0.0761  24  0.0864  25  0.0132
26  0.0114  27  0.0074  28 -0.0581  29 -0.0159  30  0.0336  31  0.0275  32  0.0073  33 -0.0020  34  0.0020  35 -0.0473
36  0.0116  37  0.0085  38  0.0159  39 -0.0125  40  0.0135

ROW  17
17  1.0000  18 -0.2633  19  0.0068  20  0.0082  21  0.0532  22  0.0759  23 -0.2456  24  0.0630  25  0.0018  26 -0.0147
27  0.0049  28 -0.0116  29 -0.0280  30  0.0421  31  0.0284  32  0.0105  33 -0.0135  34 -0.0266  35  0.0061  36 -0.0492
37  0.0324  38  0.0207  39  0.0186  40  0.0010

ROW  18
18  1.0000  19 -0.0025  20  0.0119  21  0.0004  22  0.0853  23  0.0596  24 -0.2449  25 -0.0068  26 -0.0018  27 -0.0165
28  0.0314  29  0.0373  30 -0.1135  31 -0.0126  32 -0.0078  33 -0.0012  34  0.0449  35  0.0105  36  0.0319  37 -0.0734
38 -0.0077  39 -0.0463  40  0.0001

ROW  19
19  1.0000  20 -0.0130  21 -0.0187  22 -0.0137  23  0.0091  24  0.0025  25  0.0278  26 -0.0223  27  0.0167  28 -0.0141
29 -0.0072  30  0.0008  31  0.0235  32  0.0202  33  0.0116  34 -0.0218  35  0.0040  36 -0.0083  37  0.0016  38  0.0085
39 -0.0233  40  0.0089

ROW  20
20  1.0000  21 -0.0013  22  0.0110  23 -0.0023  24 -0.0076  25 -0.0502  26  0.0036  27 -0.0156  28 -0.0328  29  0.0182
30  0.0038  31  0.0217  32 -0.0032  33  0.0169  34 -0.0015  35  0.0011  36 -0.0014  37 -0.0063  38  0.0214  39  0.0092
40 -0.0259

ROW  21
21  1.0000  22  0.0217  23 -0.0086  24  0.0015  25  0.0043  26 -0.0154  27  0.0595  28  0.0193  29 -0.0022  30  0.0173
31 -0.0238  32 -0.0083  33 -0.0610  34 -0.0398  35 -0.0130  36 -0.0204  37  0.0050  38  0.0020  39  0.0013  40  0.0354

ROW  22
22  1.0000  23 -0.2456  24 -0.2624  25 -0.0049  26  0.0378  27 -0.0050  28  0.0210  29  0.0001  30 -0.0176  31 -0.0194
32 -0.0509  33 -0.0032  34 -0.0125  35 -0.0132  36 -0.0033  37 -0.0043  38  0.0062  39  0.0042  40  0.0132

ROW  23
23  1.0000  24 -0.2504  25  0.0027  26 -0.0071  27  0.0024  28  0.0001  29  0.0103  30 -0.0178  31  0.0004  32  0.0022
33  0.0358  34  0.0449  35 -0.0080  36  0.0644  37 -0.0281  38 -0.0151  39 -0.0216  40 -0.0529

ROW  24
24  1.0000  25  0.0004  26  0.0023  27  0.0174  28 -0.0182  29 -0.0114  30  0.0530  31 -0.0011  32 -0.0040  33 -0.0075
34 -0.0382  35 -0.0024  36 -0.0284  37  0.0195  38  0.0014  39  0.0520  40  0.0127

ROW  25
25  1.0000  26  0.0192  27  0.0160  28 -0.0021  29  0.0091  30 -0.0016  31 -0.0056  32  0.0604  33 -0.0147  34 -0.0159
35 -0.0459  36 -0.0429  37  0.0176  38 -0.0132  39 -0.0226  40  0.0219
```

```
ROW  26
26  1.0000   27 -0.0134   28  0.0190   29 -0.0088   30  0.0170   31 -0.0181   32  0.0227   33 -0.0145   34  0.0307   35  0.0124
36  0.0131   37 -0.0124   38  0.0289   39  0.0028   40  0.0109

ROW  27
27  1.0000   28 -0.0020   29  0.0025   30  0.0109   31 -0.0429   32 -0.0014   33  0.0243   34 -0.0369   35  0.0108   36 -0.0368
37 -0.0021   38  0.0016   39  0.0098   40  0.0253

ROW  28
28  1.0000   29 -0.2385   30 -0.2274   31  0.0022   32 -0.0238   33  0.0023   34  0.0195   35  0.0239   36  0.0390   37  0.0002
38 -0.0126   39  0.0315   40 -0.0108

ROW  29
29  1.0000   30 -0.2553   31  0.0078   32 -0.0066   33 -0.0041   34 -0.0139   35  0.0292   36 -0.1685   37  0.0107   38 -0.0318
39 -0.0118   40  0.0233

ROW  30
30  1.0000   31  0.0020   32  0.0160   33  0.0036   34 -0.0564   35  0.0088   36  0.0050   37 -0.0059   38  0.0149   39  0.0452
40  0.0018

ROW  31
31  1.0000   32  0.0134   33 -0.0054   34 -0.0097   35 -0.0016   36 -0.0109   37  0.0116   38 -0.0055   39 -0.0054   40  0.0304

ROW  32
32  1.0000   33 -0.0249   34  0.0048   35 -0.0229   36 -0.0242   37 -0.0149   38 -0.0007   39  0.0138   40  0.0032

ROW  33
33  1.0000   34  0.0137   35  0.0004   36  0.0007   37  0.0016   38 -0.0179   39  0.0020   40 -0.0107

ROW  34
34  1.0000   35 -0.0153   36  0.0212   37  0.0251   38  0.0027   39  0.0441   40 -0.0209

ROW  35
35  1.0000   36 -0.2112   37 -0.2469   38  0.0366   39  0.0091   40 -0.0060

ROW  36
36  1.0000   37 -0.2533   38  0.0516   39 -0.0037   40  0.0346

ROW  37
37  1.0000   38 -0.0033   39 -0.0002   40  0.0163

ROW  38
38  1.0000   39  0.0362   40  0.0256

ROW  39
39  1.0000   40 -0.0280

ROW  40
40  1.0000
```

RFINE 108206 CYCLE 4

CORRELATION COEFICIENTS WITH LARGEST MAGNITUDES

PARAMETERS		VALUE	PARAMETERS		VALUE	PARAMETERS		VALUE	PARAMETERS		VALUE
1	4	-0.4804	1	3	-0.4388	1	2	-0.3722	17	18	-0.2633
22	24	-0.2624	29	30	-0.2553	11	12	-0.2545	36	37	-0.2533
23	24	-0.2504	35	37	-0.2469	16	18	-0.2462	22	23	-0.2456
17	23	-0.2456	18	24	-0.2449	28	29	-0.2385	16	22	-0.2365
15	21	-0.2351	10	11	-0.2330	10	12	-0.2275	28	30	-0.2274

RFINE 108206 CYCLE 4
BOND DISTANCES BETWEEN, 1.50 AND 2.50 ANG.

ATOM 1	X	Y	Z	ATOM 2	X	Y	Z	DISTANCE	NUMBER
M1	0.0	0.0	0.0	O1	-0.24265	0.09142	0.25000	2.18299	1
				O1	0.24265	-0.09142	-0.25000	2.18299	2
				O2	-0.28381	0.04751	-0.25000	2.14389	3
				O2	0.28381	-0.04751	0.25000	2.14389	4
				O3	0.28567	0.16253	0.04006	2.22794	5
				O3	-0.28567	-0.16253	-0.04006	2.22794	6
									7
M2	0.98766	0.28015	0.25000	O1	0.75735	0.09142	0.25000	2.29221	8
				O2	1.21619	0.45249	0.25000	2.13812	9
				O3	1.28567	0.16253	0.04006	2.31831	10
				O3	0.78567	0.33747	-0.04006	2.14658	11
				O3	0.78567	0.33747	0.54006	2.14658	12
				O3	1.28567	0.16253	0.45994	2.31831	13
									14
									15
SI	0.42650	0.09514	0.25000	O2	0.28381	-0.04751	0.25000	1.66298	5
				O3	0.28567	0.16253	0.04006	1.64119	6
				O1	0.75735	0.09142	0.25000	1.61333	9
				O3	0.28567	0.16253	0.45994	1.64119	16
									9
O1	0.75735	0.09142	0.25000	M2	0.98766	0.28015	0.25000	2.29221	8
				SI	0.42650	0.09514	0.25000	1.61333	15
				M1	1.00000	0.0	0.0	2.18299	17
				M1	1.00000	0.0	0.50000	2.18299	18
									19
O2	0.21619	0.45249	0.25000	M1	0.50000	0.50000	0.0	2.14389	20
				M1	0.50000	0.50000	0.50000	2.14389	21
				M2	-0.01234	0.28015	0.25000	2.13813	22
				SI	0.07350	0.59514	0.25000	1.66298	23
									6
O3	0.28567	0.16253	0.04006	M1	0.0	0.0	0.0	2.22794	1
				SI	0.42650	0.09514	0.25000	1.64119	15
				M2	-0.01234	0.28015	0.25000	2.31832	22
				M2	0.48766	0.21985	-0.25000	2.14658	24

RFINE 108206 CYCLE 4

BOND ANGLES

CENTRAL ATOM	X	Y	Z
M1	C.0	C.0	0.0

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
O1	2	O1	3	179.931
O1	2	O2	4	93.739
O1	2	O2	5	86.261
O1	2	O3	6	85.189
O1	2	O3	7	94.811
O1	3	O2	4	86.261
O1	3	O2	5	93.739
O1	3	O3	6	94.811
O1	3	O3	7	85.139
O2	4	O2	5	180.000
O2	4	O3	6	107.675
O2	4	O3	7	72.325
O2	5	O3	6	72.325
O2	5	O3	7	107.675
O3	6	O3	7	179.944

CENTRAL ATOM	X	Y	Z
M2	0.98766	0.28015	0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
O1	9	O2	10	177.926
O1	9	O3	11	80.711
O1	9	O3	12	91.250
O1	9	O3	13	91.250
O1	9	O3	14	80.711
O2	10	O3	11	97.586
O2	10	O3	12	89.867
O2	10	O3	13	89.867
O2	10	O3	14	97.586
O3	11	O3	12	87.927
O3	11	O3	13	156.196
O3	11	O3	14	68.740
O3	12	O3	13	114.784
O3	12	O3	14	156.196
O3	13	O3	14	87.927

CENTRAL ATOM	X	Y	Z
SI	0.42650	0.09514	0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
O2	5	O3	6	102.706
O2	5	O1	9	113.331
O2	5	O3	16	102.706
O3	6	O1	9	115.392
O3	6	O3	16	105.775
O1	9	O3	16	115.392

CENTRAL ATOM	X	Y	Z
O1	0.75735	0.09142	0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M2	8	SI	15	117.933
M2	8	M1	17	96.961
M2	8	M1	18	96.961
SI	15	M1	17	123.541
SI	15	M1	18	123.541
M1	17	M1	18	91.111

CENTRAL ATOM	X	Y	Z
O2	0.21619	0.45249	0.25000

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M1	20	M1	21	93.263
M1	20	M2	22	122.449
M1	20	SI	23	93.257
M1	21	M2	22	122.449
M1	21	SI	23	93.257
M2	22	SI	23	123.869

CENTRAL ATOM	X	Y	Z
O3	0.28567	0.16253	0.04006

ATOM 1	NUMBER	ATOM 2	NUMBER	ANGLE
M1	1	SI	15	90.859
M1	1	M2	22	94.966
M1	1	M2	24	114.252
SI	15	M2	22	92.611
SI	15	M2	24	127.071
M2	22	M2	24	127.670

RFINE 108206 CYCLE 4

ELLIPSOIDS OF VIBRATION

ELLIPSOID FOR M1

EQUIVALENT ISOTROPIC B = 0.7551

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.079546	29.96	79.13	62.46
2	0.093520	60.43	117.68	137.33
3	0.116684	94.37	149.90	60.29

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM M1 AT 0.0 0.0 0.0

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
O1	-0.24265	0.09142	0.25000	2.18299	2.18299	2.18306	2.19220	2.20141	0.09348
O1	0.24265	-0.09142	-0.25000	2.18299	2.18299	2.18306	2.19220	2.20141	0.09348
O2	-0.28381	0.04751	-0.25000	2.14389	2.14392	2.14465	2.15265	2.16137	0.09100
O2	0.28381	-0.04751	0.25000	2.14389	2.14392	2.14465	2.15265	2.16137	0.09100
O3	0.28567	0.16253	0.04006	2.22794	2.22794	2.22804	2.23643	2.24491	0.09772
O3	-0.28567	-0.16253	-0.04006	2.22794	2.22794	2.22804	2.23643	2.24491	0.09772

ELLIPSOID FOR M2

EQUIVALENT ISOTROPIC B = 0.6762

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.087003	56.24	146.24	90.00
2	0.090891	146.23	123.77	90.00
3	0.099298	90.00	90.00	0.0

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM M2 AT 0.98766 0.28015 0.25000

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
O1	0.75735	0.09142	0.25000	2.29221	2.29221	2.29253	2.30020	2.30818	0.09011
O2	1.21619	0.45249	0.25000	2.13812	2.13813	2.13839	2.14660	2.15508	0.09022
O3	1.28567	0.16253	0.04006	2.31831	2.31832	2.31871	2.32620	2.33407	0.09129
O3	0.78567	0.33747	-0.04006	2.14658	2.14663	2.14747	2.15514	2.16366	0.09607
O3	0.78567	0.33747	0.54006	2.14658	2.14663	2.14747	2.15514	2.16366	0.09607
O3	1.28567	0.16253	0.45994	2.31831	2.31832	2.31871	2.32620	2.33407	0.09129

ELLIPSOID FOR SI

EQUIVALENT ISOTROPIC B = 0.6139

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.080495	8.74	98.74	90.00
2	0.089663	98.43	171.57	90.00
3	0.093840	90.00	90.00	0.0

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM SI AT 0.42650 0.09514 0.25000

ATOM	X	Y	Z	DISTANCES RAW	LOWER	RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
O2	0.28381	-0.04751	0.25000	1.66298	1.66301	1.66374	1.67300	1.68299	0.08901
O3	0.28567	0.16253	0.04006	1.64119	1.64132	1.64284	1.65207	1.66283	0.09038
O1	0.75735	0.09142	0.25000	1.61333	1.61371	1.61652	1.62695	1.64019	0.08065
O3	0.28567	0.16253	0.45994	1.64119	1.64132	1.64284	1.65207	1.66283	0.09038

ELLIPSOID FOR O1

EQUIVALENT ISOTROPIC B = 0.8072

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.059516	0.90	90.90	90.00
2	0.114731	90.00	90.00	180.00
3	0.118164	89.10	0.90	90.00

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O1 AT 0.75735 0.09142 0.25000

ATOM	X	Y	Z	DISTANCES RAW	LOWER	RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
M2	0.98766	0.28015	0.25000	2.29221	2.29221	2.29253	2.30020	2.30818	0.10771
SI	0.42650	0.09514	0.25000	1.61333	1.61371	1.61652	1.62695	1.64019	0.05952
M1	1.00000	0.0	0.0	2.18299	2.18299	2.18306	2.19220	2.20141	0.10206
M1	1.00000	0.0	0.50000	2.18299	2.18299	2.18306	2.19220	2.20141	0.10206

ELLIPSOID FOR O2

EQUIVALENT ISOTROPIC B = 0.6897

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.082290	15.42	74.57	90.00
2	0.091267	74.57	164.57	90.00
3	0.105374	90.00	90.00	0.0

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O2 AT 0.21619 0.45249 0.25000

ATOM	X	Y	Z	DISTANCES RAW	LOWER	RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
M1	0.50000	0.50000	0.0	2.14389	2.14392	2.14465	2.15265	2.16137	0.09521
M1	0.50000	0.50000	0.50000	2.14389	2.14392	2.14465	2.15265	2.16137	0.09521
M2	-0.01234	0.28015	0.25000	2.13813	2.13813	2.13840	2.14660	2.15508	0.08661
SI	0.07350	0.59514	0.25000	1.66298	1.66301	1.66374	1.67300	1.68299	0.09104

ELLIPSOID FOR O3

EQUIVALENT ISOTROPIC B = 0.7714

AXIS	RMS AMPLITUDE	ANGLE WITH A	ANGLE WITH B	ANGLE WITH C
1	0.093077	62.97	125.36	47.38
2	0.095089	28.17	82.22	116.89
3	0.107722	80.30	36.61	55.10

RMS DISPLACEMENTS AND THERMAL CORRECTIONS TO BONDS FROM O3 AT 0.28567 0.16253 0.04006

ATOM	X	Y	Z	RAW	LOWER	DISTANCES RIDING	NON-CORR	UPPER	DISPLACEMENT ALONG BOND
M1	0.0	0.0	0.0	2.22794	2.22794	2.22804	2.23643	2.24491	0.10314
SI	0.42650	0.09514	0.25000	1.64119	1.64132	1.64284	1.65207	1.66283	0.09357
M2	-0.01234	0.28015	0.25000	2.31832	2.31833	2.31871	2.32620	2.33408	0.10052
M2	0.48766	0.21985	-0.25000	2.14658	2.14663	2.14747	2.15514	2.16365	0.09496

PARAMETERS WRITTEN OUT TO UNIT 10.

SUMMARY OF ERRORS FOR THIS JOB	ERROR NUMBER	NUMBER OF ERRORS
	209	1

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HASP JOB NO. = 1999    SYSTEM ENTRY        TIME = 11.10.42   DATE = SEP 14, 1979
                              PURGE               11.29.54          SEP 14, 1979

    B0020CAF   310D3

JOB ACCOUNTING SUMMARY      START TIME ON MAIN    11.16.29

    EXECUTION TIME ON CPU1                         00.00.36            2.00
    DISK EXCPS                                          527             .13
    TAPE EXCPS                                            0             .00
    KILOBYTE SECONDS                                  34352             .67

    CARD INPUT ON READER2                                60             .09

    CARDS PUNCHED
       LOCAL                                             15             .07

    LINES PRINTED
       LOCAL                                           3203            2.24

    PLOTTER CHARGES

    PRIORITY CHARGES
                                              STANDARD EXECUTION        .00
                                              STANDARD OUTPUT           .00
    SETUPS

    TOTAL RUN CHARGES                                                  5.20

CURRENT BALANCE                                                      390.93
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